

Decision Theory

Performance evaluation review

Metrics & Evaluation

(regression/classification metrics, ROC curves)

Quantify model performance

Experimental Design

Set of decisions to fairly compare models to determine what impacts model performance

Model Comparison

Fairly **compare** model generalization performance

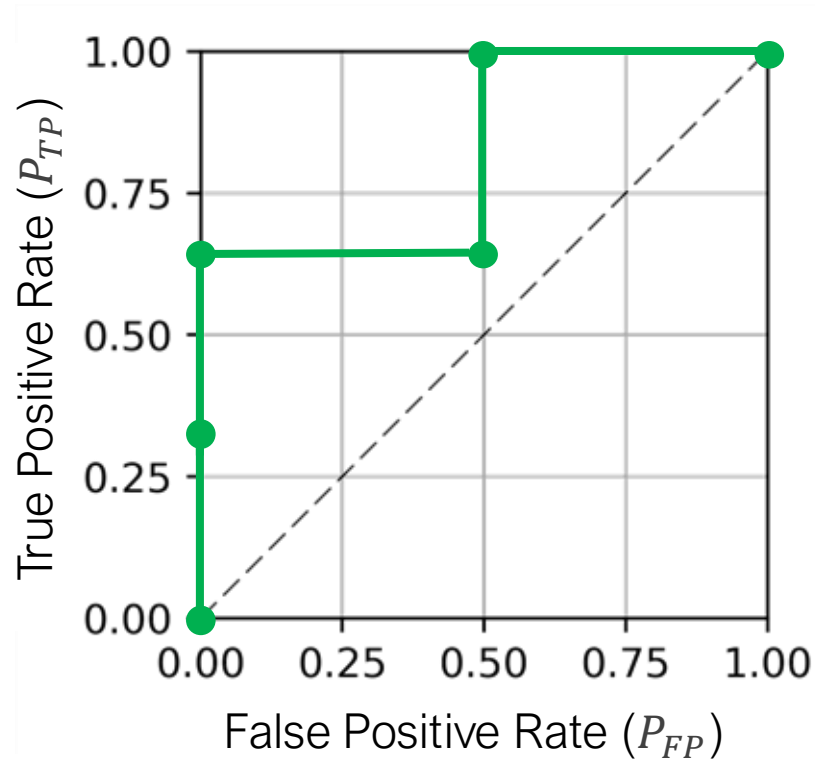
Performance Evaluation

Estimate generalization performance



Performance Evaluation → Application

How do we use this information...



→ ...to make practical predictions?

Time to make a decision...

Exercise inspired by Mausam, University of Washington, CSE573

State of Nature

Poor market
performance

Good market
performance

Payoff

Payoff

Buy Apple

-1,000

1,700

-10% to
+17% return

Buy Google

-2,000

2,100

-20% to
+21% return

Buy bonds

500

500

Guaranteed
5% return

How to invest \$10,000?

Maximax

Optimism

Select the maximum of the maximum payoff

Action

	State of Nature		Criterion
	Poor market performance Payoff	Good market performance Payoff	Maximum payoff for an action
Buy Apple	-1,000	1,700	1,700
Buy Google	-2,000	2,100	2,100
Buy bonds	500	500	500

← **Maximax**

Maximin

Pessimism

Select the maximum of the minimum payoffs

Action

State of Nature

Criterion

Poor market
performance

Good market
performance

Minimum
payoff for an
action

Payoff

Payoff

Buy Apple

-1,000

1,700

-1,000

Buy Google

-2,000

2,100

-2,000

Buy bonds

500

500

500



Maximin

Minimax

Select the minimum maximum regret

Action

		State of Nature				Criterion
		Poor market performance	Good market performance			Maximum regret for an action
		Payoff	Regret	Payoff	Regret	
Buy Apple		-1,000	1,500	1,700	400	1,500
Buy Google		-2,000	2,500	2,100	0	2,500
Buy bonds		500	0	500	1,600	1,600

←
Minimax

Which decision would I regret least?

Regret = Opportunity Loss
Difference between a decision made and an optimal decision

Next: factor in probabilities of different outcomes

Expected Payoff: Equal likelihood

Action	State of Nature		Criterion	Select the highest average payoff ASSUMING all states are of equal probability
	Poor market performance	Good market performance	Expected reward/ payoff	
	Payoff	Payoff		
Buy Apple	-1,000	1,700	350	← Maximum Expected Reward
Buy Google	-2,000	2,100	50	
Buy bonds	500	500	500	
State Probability:	0.5	0.5		

Expected Payoff

Action	State of Nature		Criterion	Select the highest average payoff assuming state probabilities from prior knowledge	← Maximum Expected Reward
	Poor market performance	Good market performance	Expected reward/ payoff		
	Payoff	Payoff			
	0.3	0.7			
Buy Apple	-1,000	1,700	890		
Buy Google	-2,000	2,100	870		
Buy bonds	500	500	500		

Decision making design pattern

1. Define a measure of risk or reward
2. Select the action that optimizes that metric

Notation

$$EV(a_i) = \lambda(a_i|s_0)P(s_0) + \lambda(a_i|s_1)P(s_1)$$

↑
Expected reward

State of Nature (s)

Action	State of Nature (s)		Expected Reward $EV(a_i)$
	Poor market performance $s = s_0$	Excellent market performance $s = s_1$	
	$\lambda(a_0 s_0)$ -1,000	$\lambda(a_0 s_1)$ 1,700	
	$\lambda(a_1 s_0)$ -2,000	$\lambda(a_1 s_1)$ 2,100	
Buy Apple $a = a_0$			$(0.3)(-1000) + (0.7)(1700)$ = 890
Buy Google $a = a_1$			$(0.3)(-2000) + (0.7)(2100)$ = 870
Buy bonds $a = a_2$	$\lambda(a_2 s_0)$ 500	$\lambda(a_2 s_1)$ 500	$(0.3)(500) + (0.7)(500)$ = 500

State Probability: $P(s_0) = 0.3$ $P(s_1) = 0.7$

Risk = expected loss (cost)

Loss: $\lambda(a_i | s_j) \triangleq$ Loss incurred by choosing action i and the state of nature being state j

Risk:
Expected loss $R(a_i) = \sum_{j=1}^{N_s} \lambda(a_i | s_j) P(s_j)$

Goal: Select action i for which $R(a_i)$ is minimum

Payoff

State of Nature

Poor market performance Good market performance

Action	Buy Apple	-1,000	1,700
	Buy Google	-2,000	2,100
	Buy bonds	500	500

Loss

(here we define loss in terms of opportunity cost)

State of Nature

Poor market performance Good market performance

Action	Buy Apple	1,500	400
	Buy Google	2,500	0
	Buy bonds	0	1,600

Investments: loss

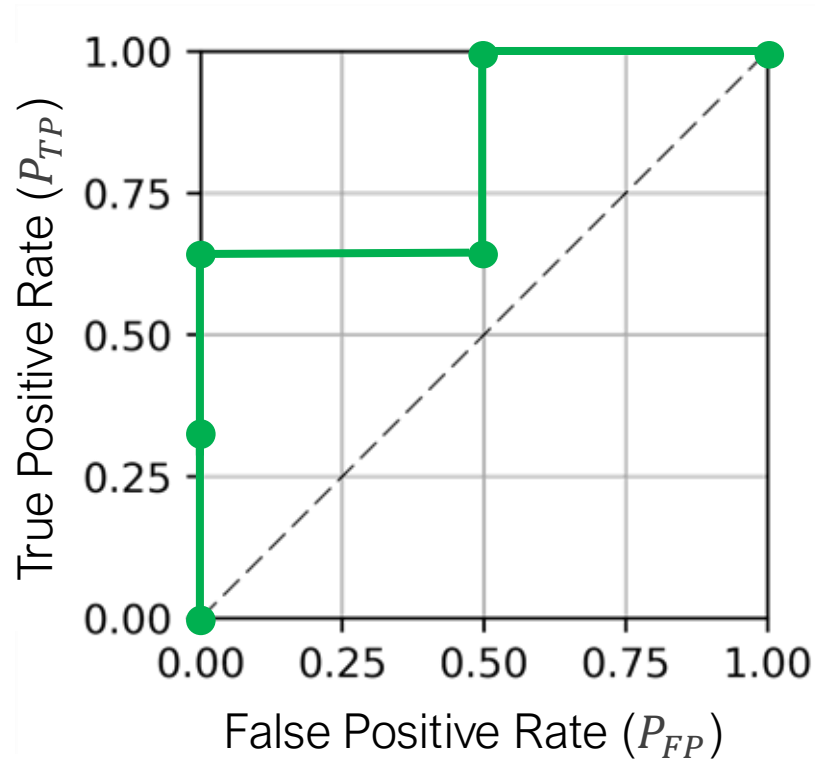
$$R(a_i) = \lambda(a_i|s_0)P(s_0) + \lambda(a_i|s_1)P(s_1)$$

↑
Risk (Expected loss)

		State of Nature (s)		Risk (Expected Loss) $R(a_i)$
		Poor market performance $s = s_0$	Excellent market performance $s = s_1$	
Action	Buy Apple $a = a_0$	$\lambda(a_0 s_0)$ 1,500	$\lambda(a_0 s_1)$ 400	$(0.3)(1500) + (0.7)(400)$ = 730
	Buy Google $a = a_1$	$\lambda(a_1 s_0)$ 2,500	$\lambda(a_1 s_1)$ 0	$(0.3)(2500) + (0.7)(0)$ = 750
	Buy bonds $a = a_2$	$\lambda(a_2 s_0)$ 0	$\lambda(a_2 s_1)$ 1,600	$(0.3)(0) + (0.7)(1600)$ = 1220
State Probability:		$P(s_0) = 0.3$	$P(s_1) = 0.7$	

We can use risk to choose where to operate along an ROC curve

Performance Evaluation → Application



The "actions" we can evaluate here are which point along the ROC curve to operate?

In other words – what **threshold do I pick** for my classifier decision rule?

↖
action

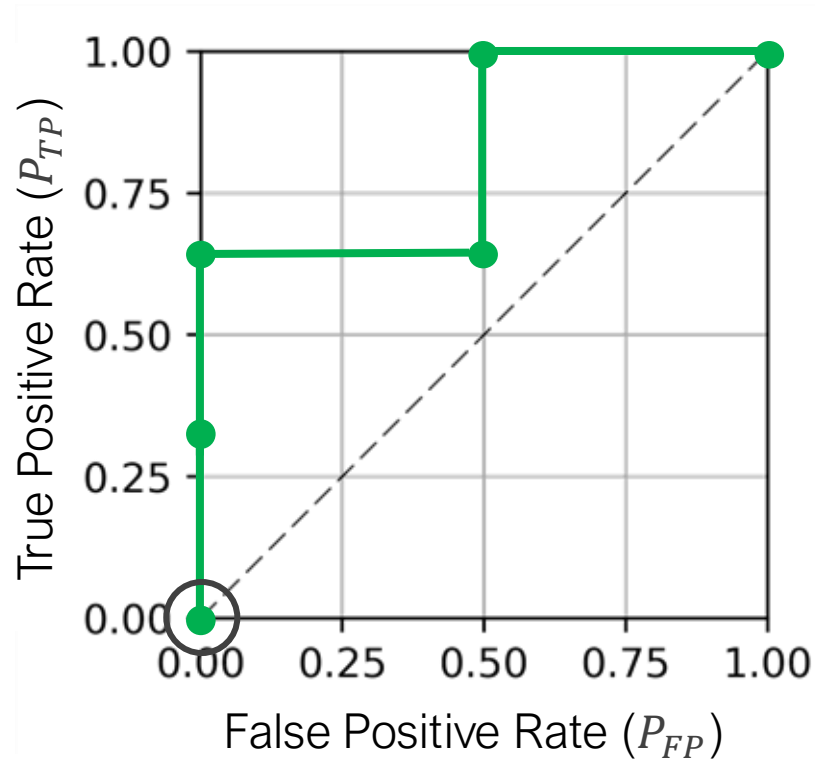
Classifier decision rule:

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

Note: we define: $\tau \equiv \text{thresh}$

Performance Evaluation → Application

Each point along the ROC represents a different confusion matrix and different rates for TP, FP, TN, FN



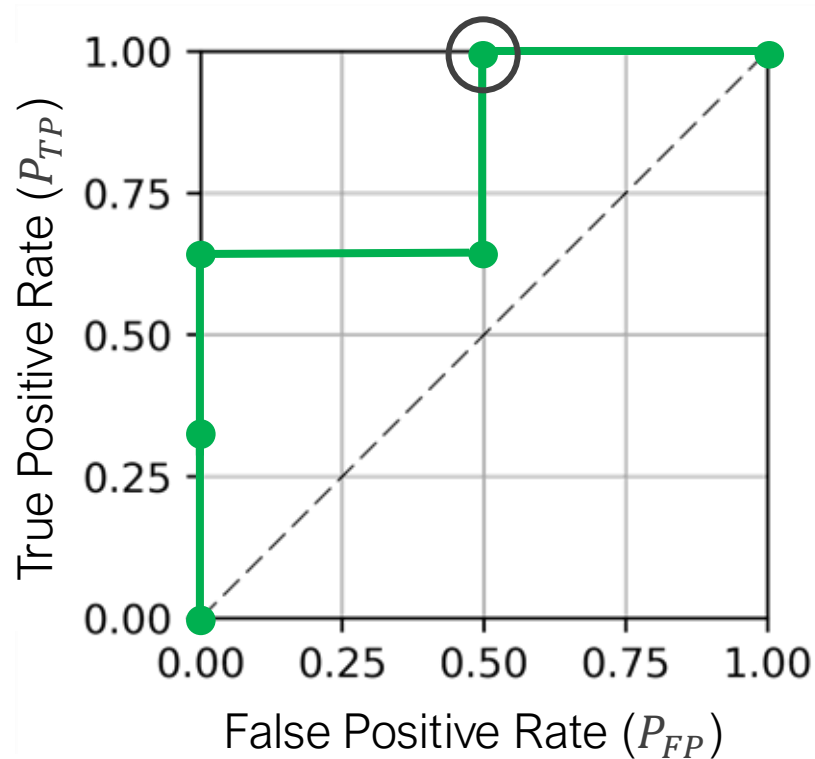
Raw values

Predicted Class			
True Class	Class 1	Class 0	
Class 1	TP 0	FN 50	[50]
Class 0	FP 0	TN 50	[50]

Rates / probabilities

Predicted Class			
True Class	Class 1	Class 0	
Class 1	TPR 0	FNR 1.0	[50]
Class 0	FPR 0	TNR 1.0	[50]

Performance Evaluation → Application



Each point along the ROC represents a different confusion matrix and different rates for TP, FP, TN, FN

Raw values

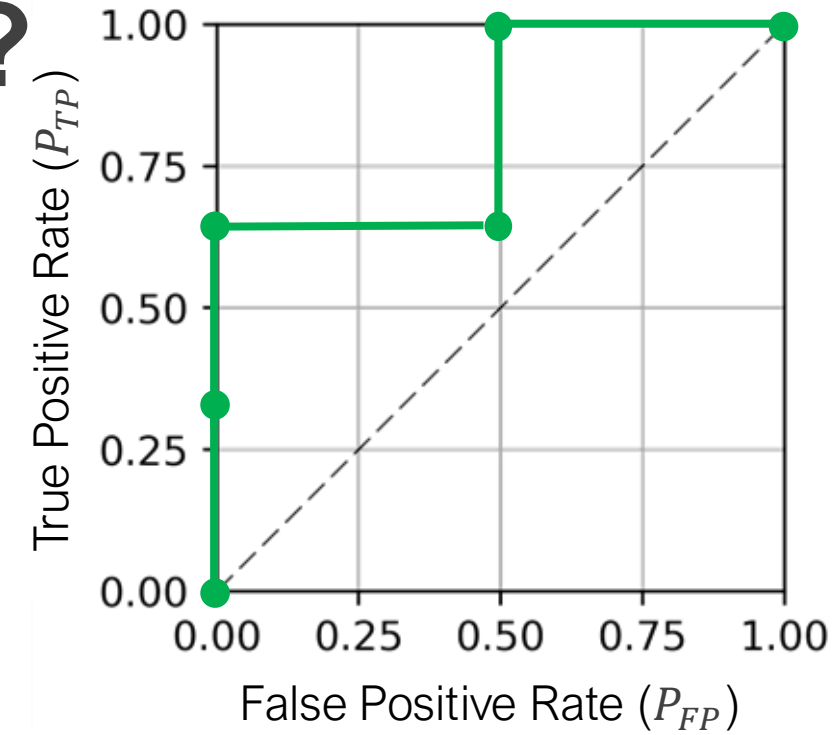
		Predicted Class		
		Class 1	Class 0	
True Class	Class 1	TP 50	FN 0	[50]
	Class 0	FP 25	TN 25	[50]

Rates / probabilities

		Predicted Class		
		Class 1	Class 0	
True Class	Class 1	TPR 1.0	FNR 0	[50]
	Class 0	FPR 0.5	TNR 0.5	[50]

Where to operate along ROC?

		Estimate	
		Class 1	Class 0
Truth	Class 1	True Positive $\lambda_{11} = \mathbf{0}$	False negative $\lambda_{01} = \mathbf{100}$
	Class 0	False Positive $\lambda_{10} = \mathbf{1}$	True Negative $\lambda_{00} = \mathbf{0}$



$$\lambda_{ij} = \lambda(\hat{y} = i, y = j)$$

Loss if prediction is class i when truth is class j

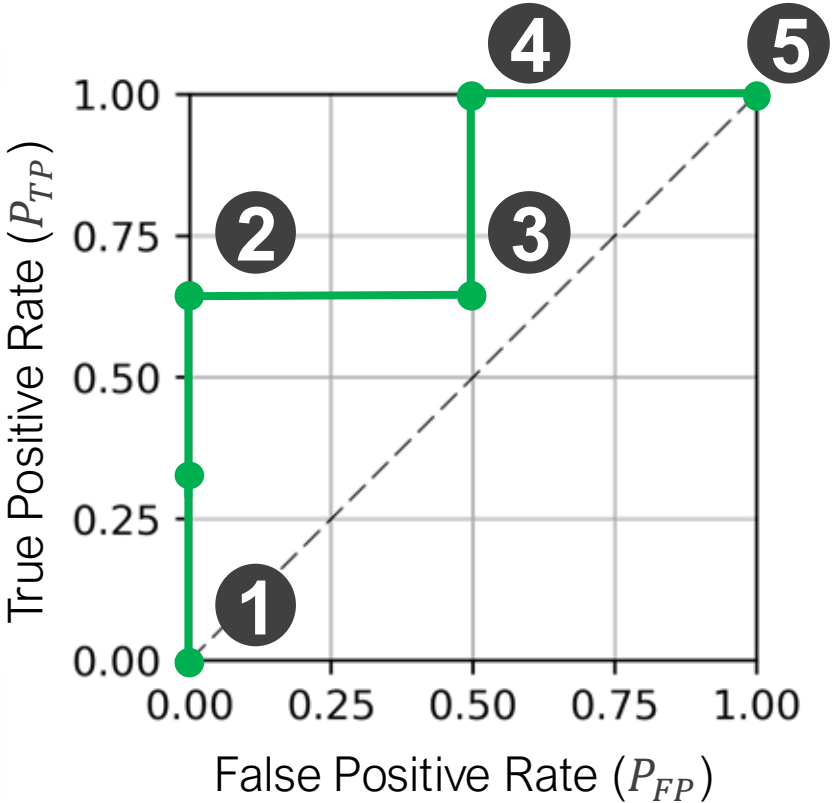
- Assume for our problem a false negative is 100 times worse than a false positive
- Correct predictions incur no penalties

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1			
2			
3			
4			
5			

$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k)$$

$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) + \lambda_{01} P_{FN}(\tau_k)$$



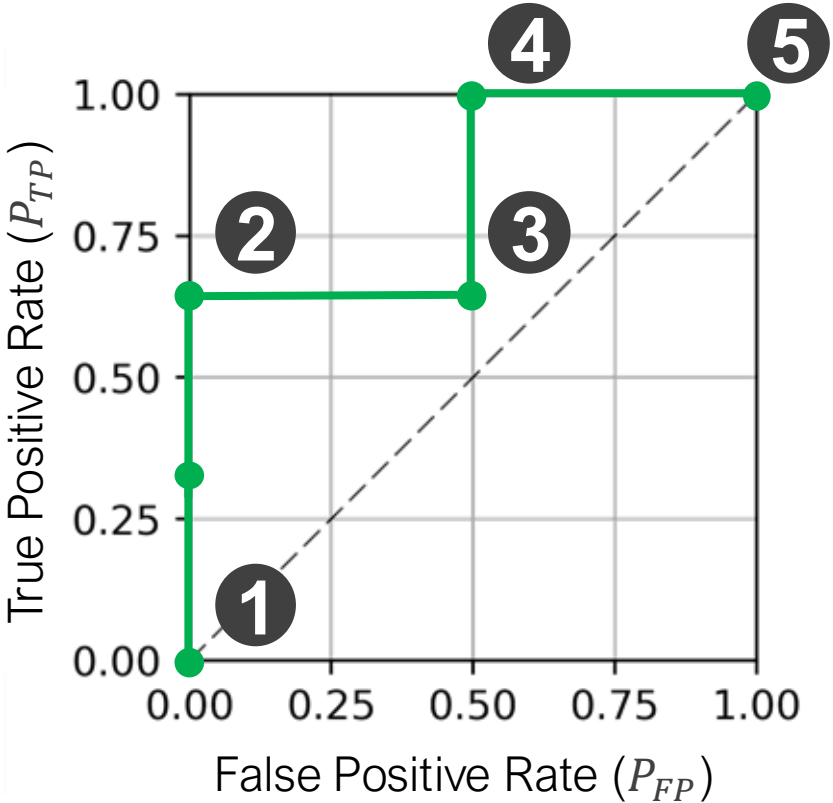
		Estimate	
		Class 1	Class 0
Truth	Class 1	True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
	Class 0	False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1	0	1	100
2			
3			
4			
5			

$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k)$$

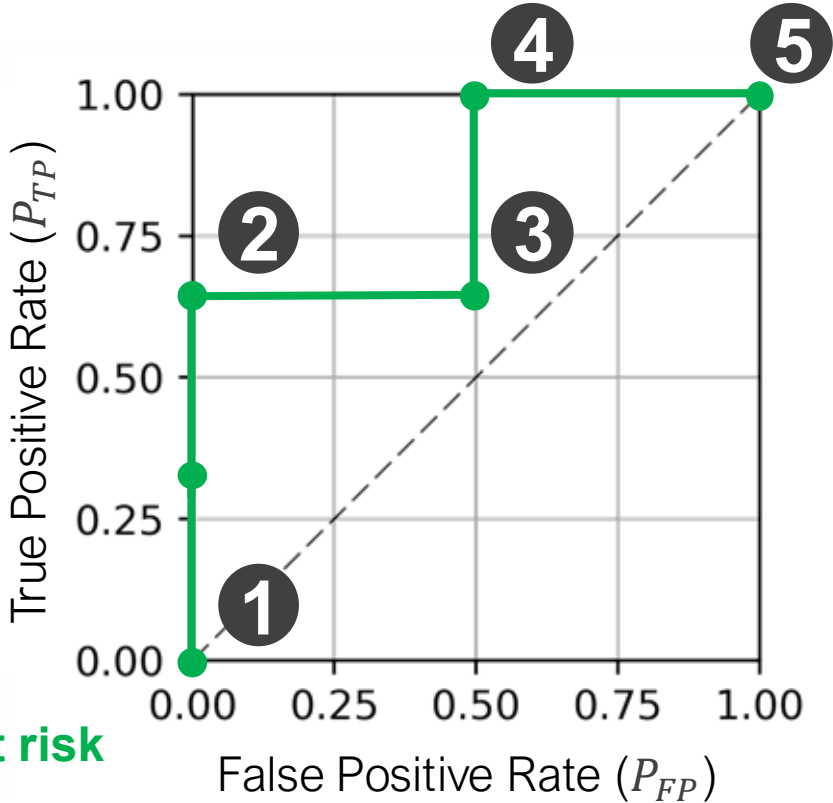
$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) + \lambda_{01} P_{FN}(\tau_k)$$



		Estimate	
		Class 1	Class 0
Truth	Class 1	True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
	Class 0	False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1	0	1	100
2	0	0.33	33
3	0.5	0.33	33.5
4	0.5	0	0.5
5	1	0	1



$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k)$$

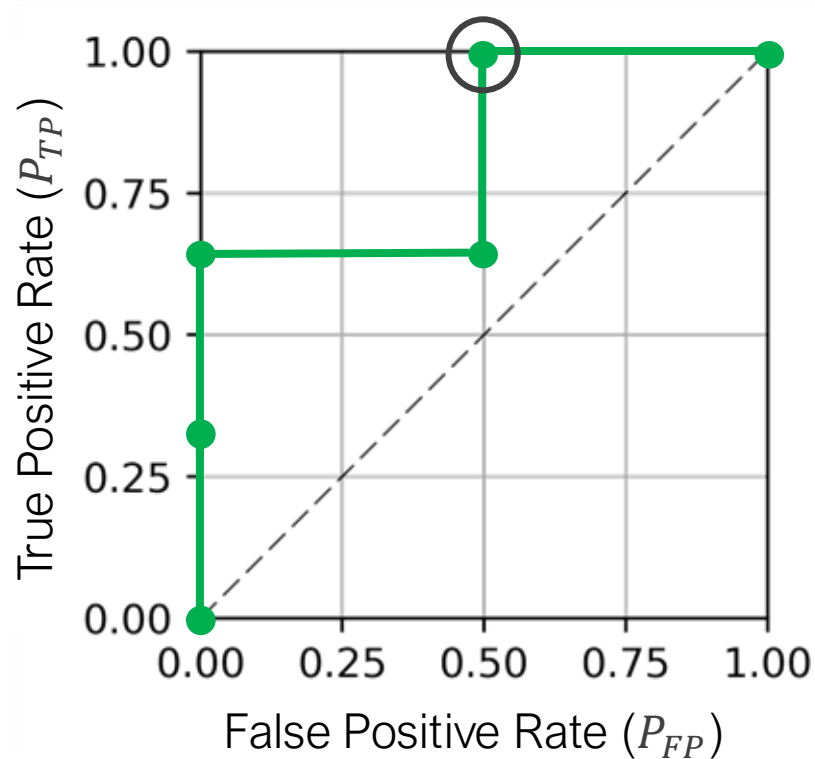
$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) + \lambda_{01} P_{FN}(\tau_k)$$

		Estimate	
		Class 1	Class 0
Truth	Class 1	True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
	Class 0	False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$

This makes a critical assumption about how the data are distributed by class...

Note: in the previous examples, if we wanted risk to equal expected loss, we would need to have assigned a probability of 0.5 to each class

Performance Evaluation → Application



Each point along the ROC represents a different confusion matrix and different rates for TP, FP, TN, FN

Raw values

		Predicted Class		
		Class 1	Class 0	
True Class	Class 1	TP 50	FN 0	[50]
	Class 0	FP 25	TN 25	[50]

Rates / probabilities

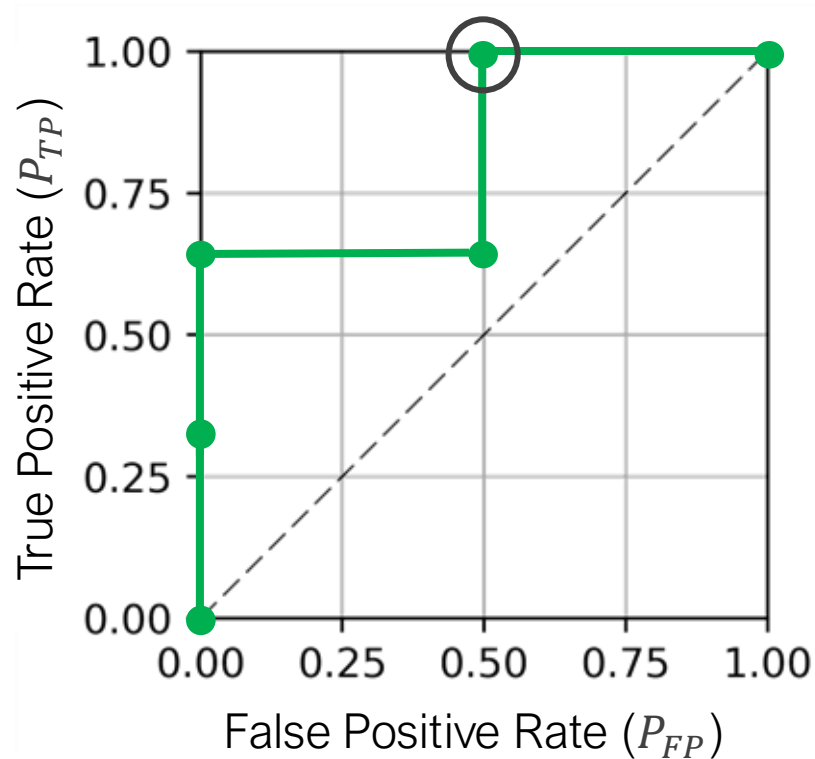
		Predicted Class		
		Class 1	Class 0	
True Class	Class 1	TPR 1.0	FNR 0	[50]
	Class 0	FPR 0.5	TNR 0.5	[50]

$$\text{Precision} = 50 / 75 = 0.67$$

Classes are equiprobable
 $P(Y = 1) = P(Y = 0) \cong 0.5$

Performance Evaluation → Application

Each point along the ROC represents a different confusion matrix and different rates for TP, FP, TN, FN



Raw values

Predicted Class			
True Class	Class 1	Class 0	
Class 1	TP 5	FN 0	[5]
Class 0	FP 25	TN 25	[50]

$$\text{Precision} = 5 / 30 = 0.17$$

Rates / probabilities

Predicted Class			
True Class	Class 1	Class 0	
Class 1	TPR 1.0	FNR 0	[5]
Class 0	FPR 0.5	TNR 0.5	[50]

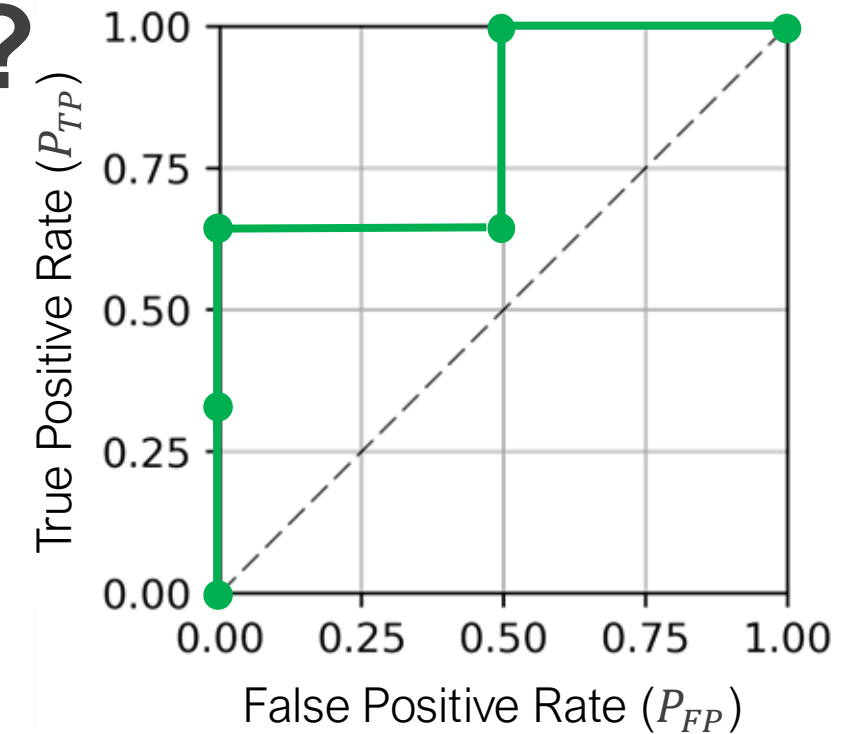
$$P(Y = 1) \cong \frac{5}{55} = 0.09$$
$$P(Y = 0) \cong \frac{50}{55} = 0.89$$

ROC curves are not sensitive to class imbalances – TPR and FPR are class-conditional

This means we need to factor in the prevalence of each class

Where to operate along ROC?

		Estimate	
		Class 1	Class 0
Truth	Class 1 $\pi_1 = P(Y = 1)$	True Positive $\lambda_{11} = \mathbf{0}$	False negative $\lambda_{01} = \mathbf{100}$
	Class 0 $\pi_0 = P(Y = 0)$	False Positive $\lambda_{10} = \mathbf{1}$	True Negative $\lambda_{00} = \mathbf{0}$



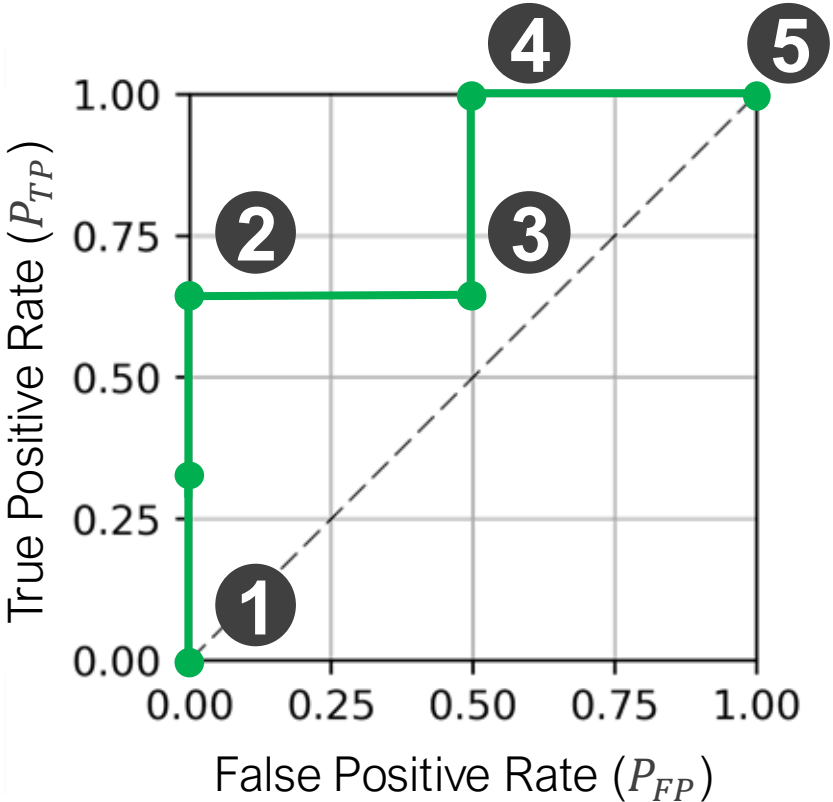
$$\lambda_{ij} = \lambda(\hat{y} = i, y = j)$$

Loss if prediction is class i when truth is class j

Class prevalence also needs to be factored in!

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1	0	1	1
2	0	0.33	
3	0.5	0.33	
4	0.5	0	
5	1	0	



$P(Y = 0) \cong 0.99$
 $P(Y = 1) \cong 0.01$

Estimate

$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k) P(Y = j)$$

$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) \pi_0 + \lambda_{01} P_{FN}(\tau_k) \pi_1$$

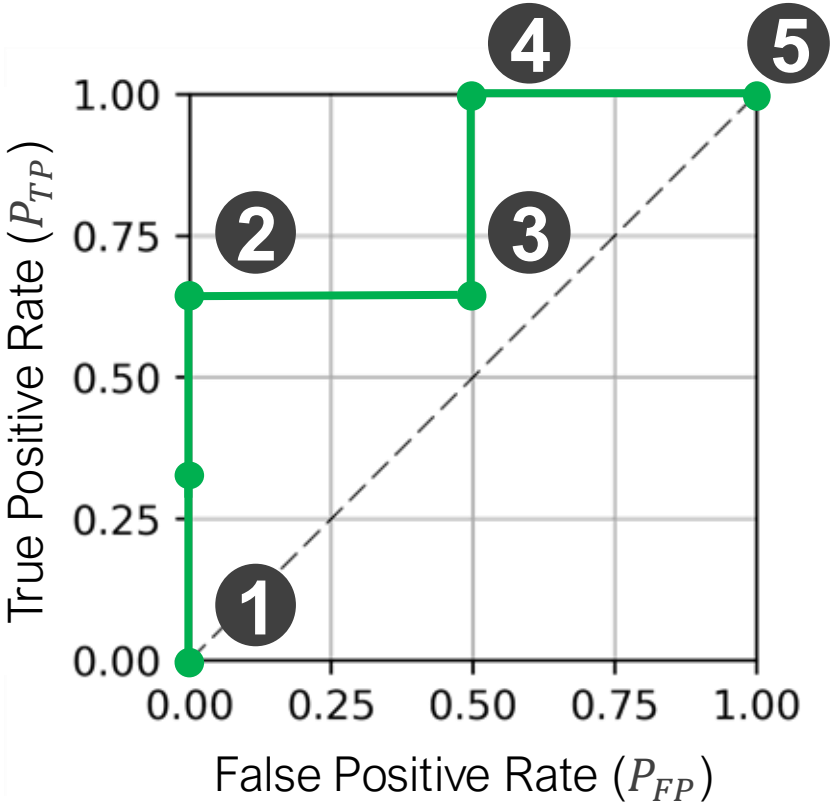
$$\pi_i = P(Y = i)$$

Truth

	Class 1	Class 0
Class 1	True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
Class 0	False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1	0	1	1
2	0	0.33	0.33
3	0.5	0.33	
4	0.5	0	
5	1	0	



$P(Y = 0) \cong 0.99$
 $P(Y = 1) \cong 0.01$

Estimate

	Class 1	Class 0
Truth	Class 1	Class 0
	Class 0	Class 1

$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k) P(Y = j)$$

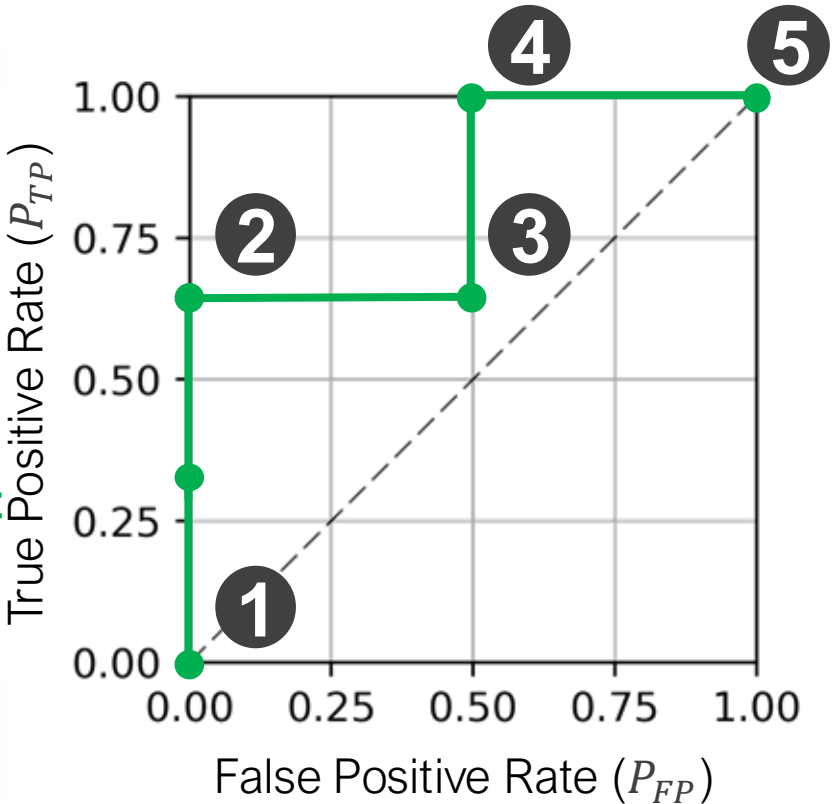
$\pi_i = P(Y = i)$

$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) \pi_0 + \lambda_{01} P_{FN}(\tau_k) \pi_1$$

Choose where to operate

Action: select threshold	Probability of false positive	Probability of false negative	Risk
k	P_{FP}	$P_{FN} = (1 - P_{TP})$	$R(\tau_k)$
1	0	1	1
2	0	0.33	0.33
3	0.5	0.33	0.83
4	0.5	0	0.50
5	1	0	0.99

Least risk



$P(Y = 0) \cong 0.99$
 $P(Y = 1) \cong 0.01$

Estimate

Class 1 Class 0

Truth

Class 1	True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
Class 0	False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$

$$R(\tau_k) = \sum_{i,j} \lambda(\hat{y} = i, y = j) P(\hat{Y} = i | Y = j, \tau_k) P(Y = j)$$

$$\pi_i = P(Y = i)$$

$$R(\tau_k) = \lambda_{10} P_{FP}(\tau_k) \pi_0 + \lambda_{01} P_{FN}(\tau_k) \pi_1$$

Takeaways

Models make predictions, but these need to be contextualized to transform them into a decision

To make a decision, we minimize expected loss (risk):

1. Define a measure of risk
2. Select the action that optimizes that metric (for binary classification, this is often the decision rule threshold)

Decision theory systematically incorporates the relative importance of different error types and the prevalence of the types of classes

Requires application domain knowledge to reflect real-world importance