

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

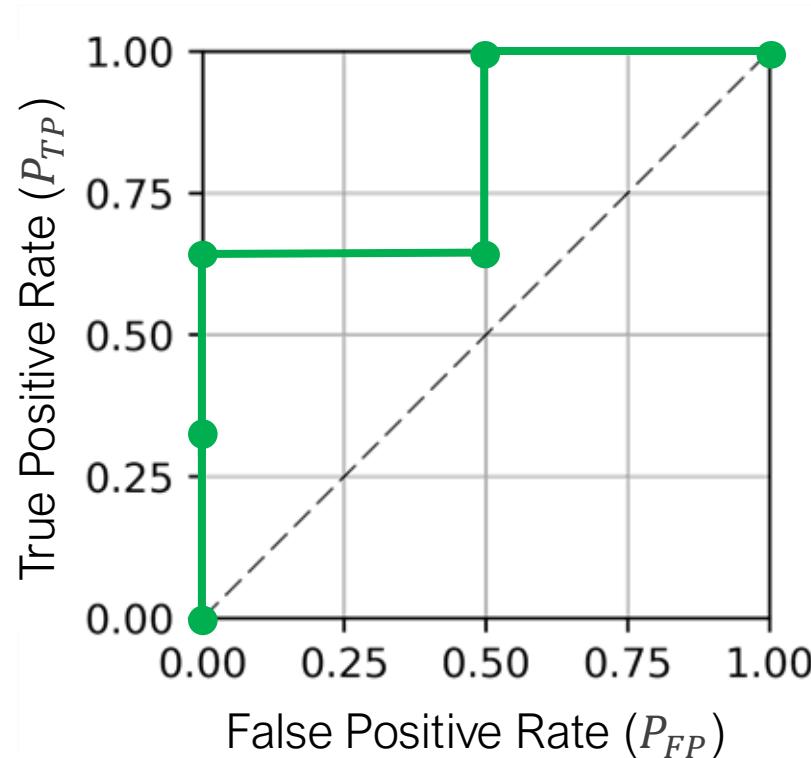
Fairly **compare** model generalization performance

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

Action

Buy Apple

Buy Google

Buy bonds

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

Optimism

Select the maximum of the maximum payoff

← **Maximax**

Maximin

Action	State of Nature		Criterion
	Poor market performance	Good market performance	
	Payoff	Payoff	
Buy Apple	-1,000	1,700	-1,000
Buy Google	-2,000	2,100	-2,000
Buy bonds	500	500	500

Pessimism

Select the maximum of the minimum payoffs

← **Maximin**

Minimax

Select the minimum maximum regret

State of Nature

Criterion

Maximum regret for an action

Poor market performance Good market performance

Payoff

Regret

Payoff

Regret

Buy Apple

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

Maximum Expected Reward

←

State Probability: 0.5 0.5

Expected Payoff

Action	State of Nature		Criterion Expected reward/ payoff
	Poor market performance	Good market performance	
Payoff	Payoff		
Buy Apple	-1,000	1,700	890
Buy Google	-2,000	2,100	870
Buy bonds	500	500	500

State Probability: 0.3 0.7

Select the highest average payoff assuming state probabilities from prior knowledge

←

Maximum Expected Reward

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

Loss

(here we define loss in terms of opportunity cost)

State of Nature

	Poor market performance	Good market performance
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Buy Apple	-1,000	1,700
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Buy Google	-2,000	2,100
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Buy bonds	500	500
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Action

Buy Apple	1,500	400
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Buy Google	2,500	0
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Buy bonds	0	1,600
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State of Nature

	Poor market performance	Good market performance
--	-------------------------	-------------------------

Buy Apple	1,500	400
-----------	-------	-----

Buy Google	2,500	0
------------	-------	---

Buy bonds	0	1,600
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Investments: loss

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

↑
Risk (Expected loss)

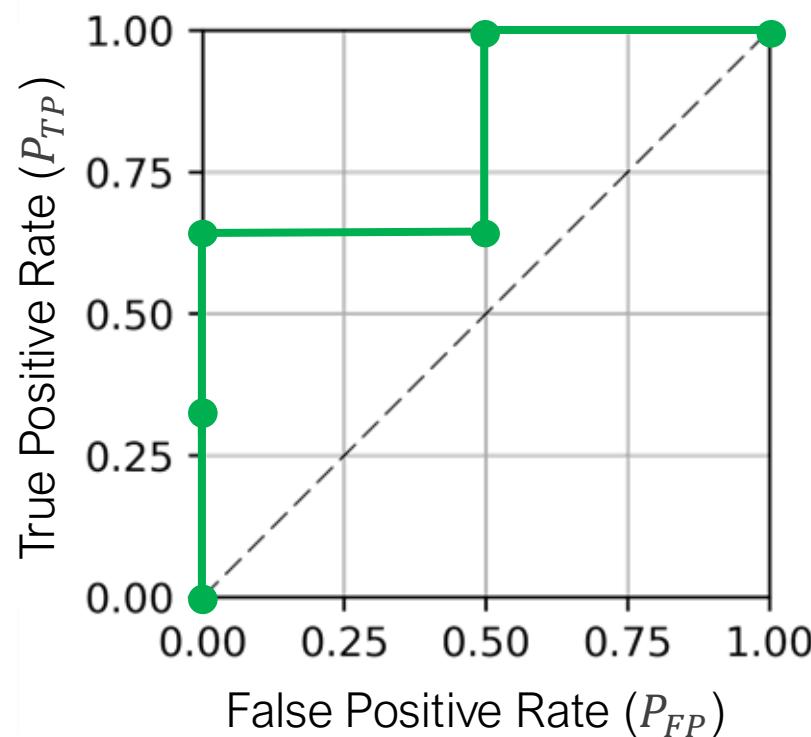
	State of Nature (s)		Risk (Expected Loss) $R(a_i)$
	Poor market performance $s = s_0$	Excellent market performance $s = s_1$	
Action			
Buy Apple $a = a_0$	$\lambda(a_0 s_0)$ 1,500	$\lambda(a_0 s_1)$ 400	$(0.3)(1500) + (0.7)(400)$ = 730
Buy Google $a = a_1$	$\lambda(a_1 s_0)$ 2,500	$\lambda(a_1 s_1)$ 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?

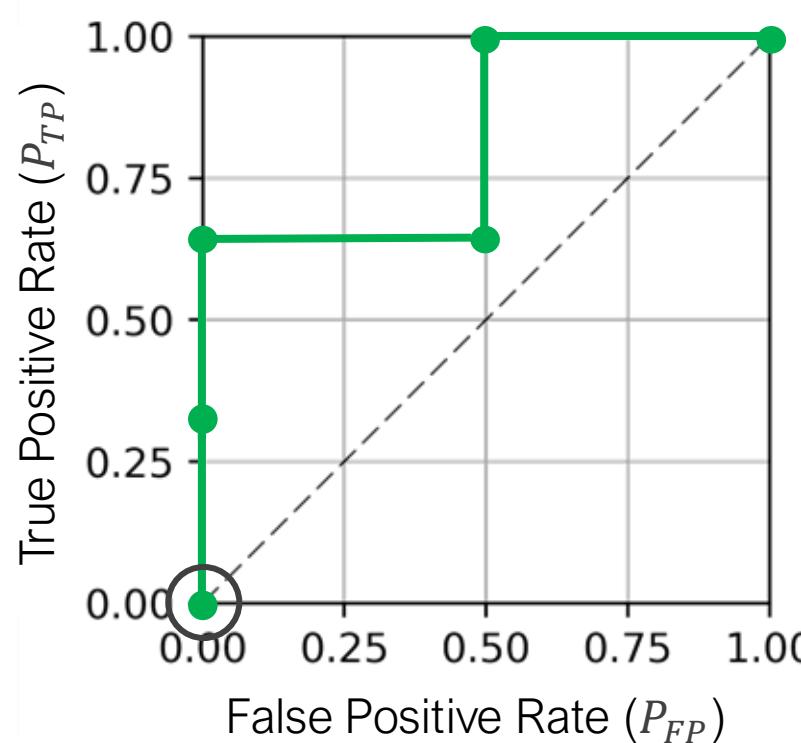
action

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

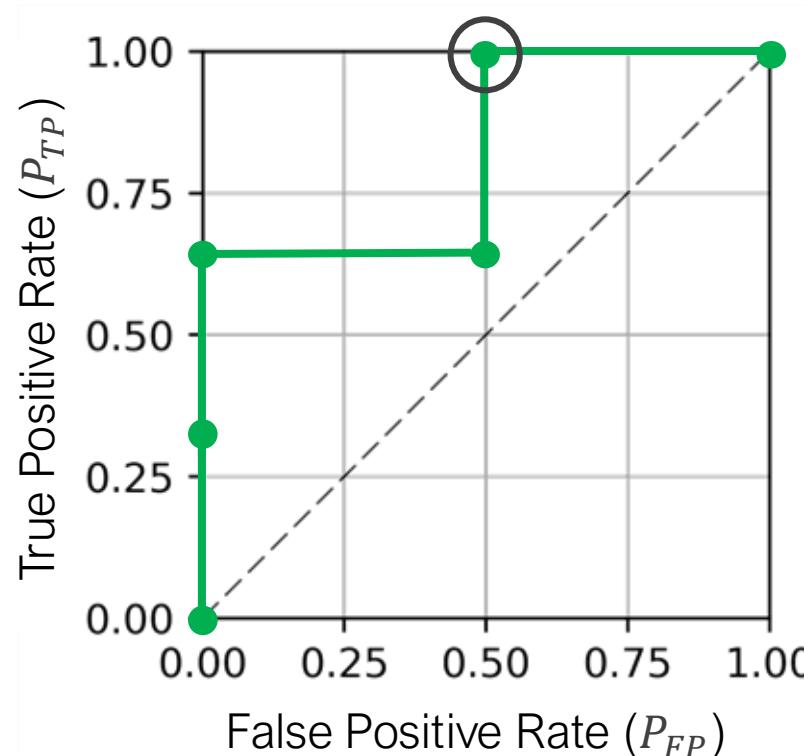
Raw values

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

Rates / probabilities

		Predicted Class		
		Class 1	Class 0	
True Class	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

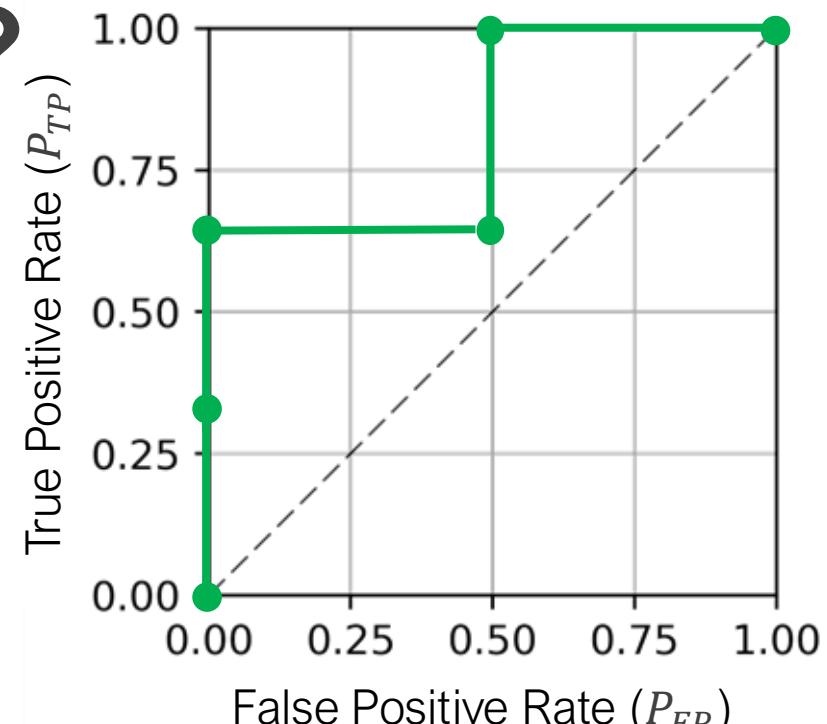
		Predicted Class		
		Class 1	Class 0	
True Class	Class 1	TP 50	FN 0	[50]
	Class 0	FP 25	TN 25	[50]

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



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

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

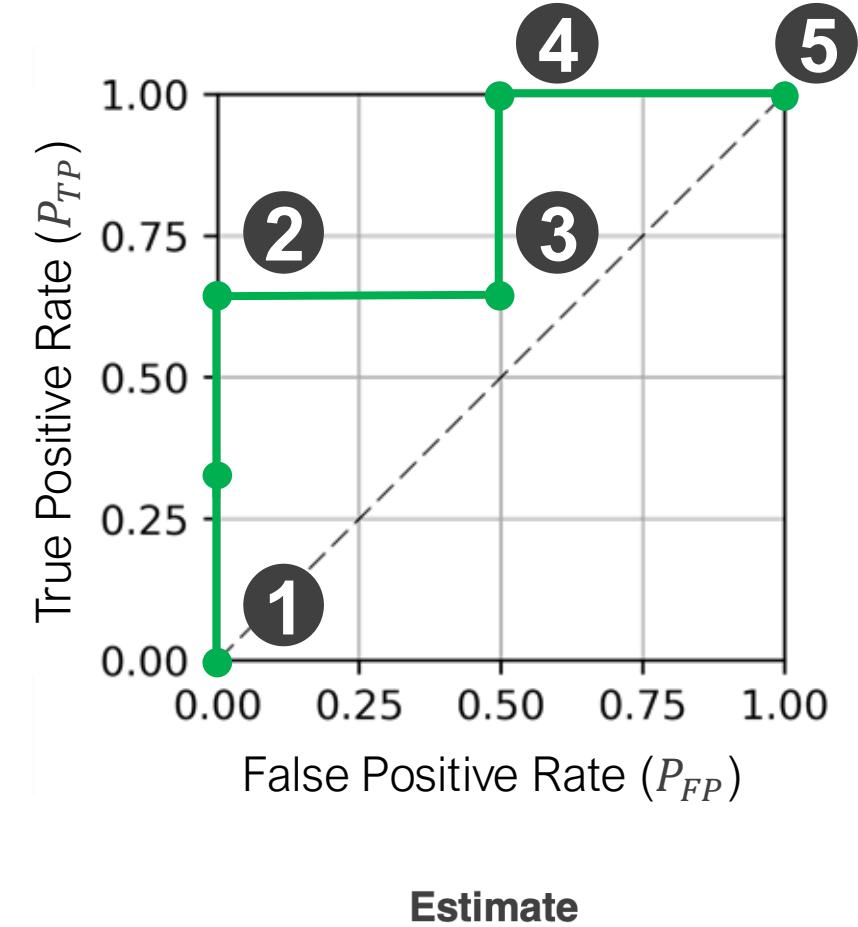
Choose where to operate

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

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

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

Truth



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

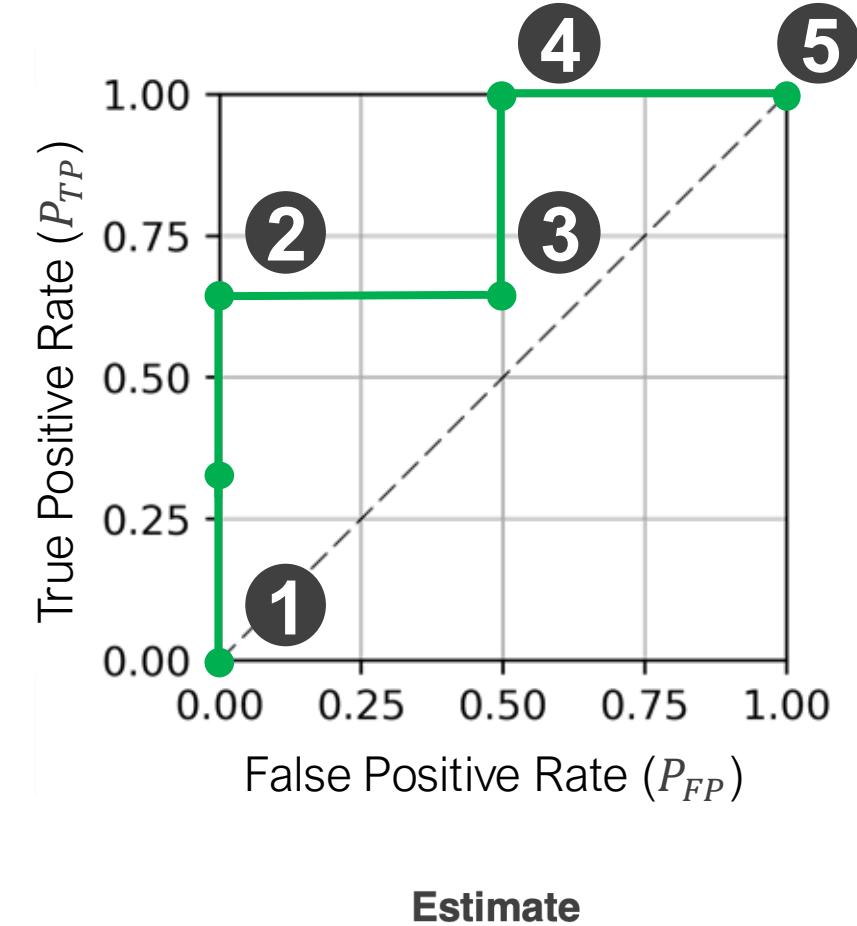
Choose where to operate

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

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

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

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 $\lambda_{00} = 0$

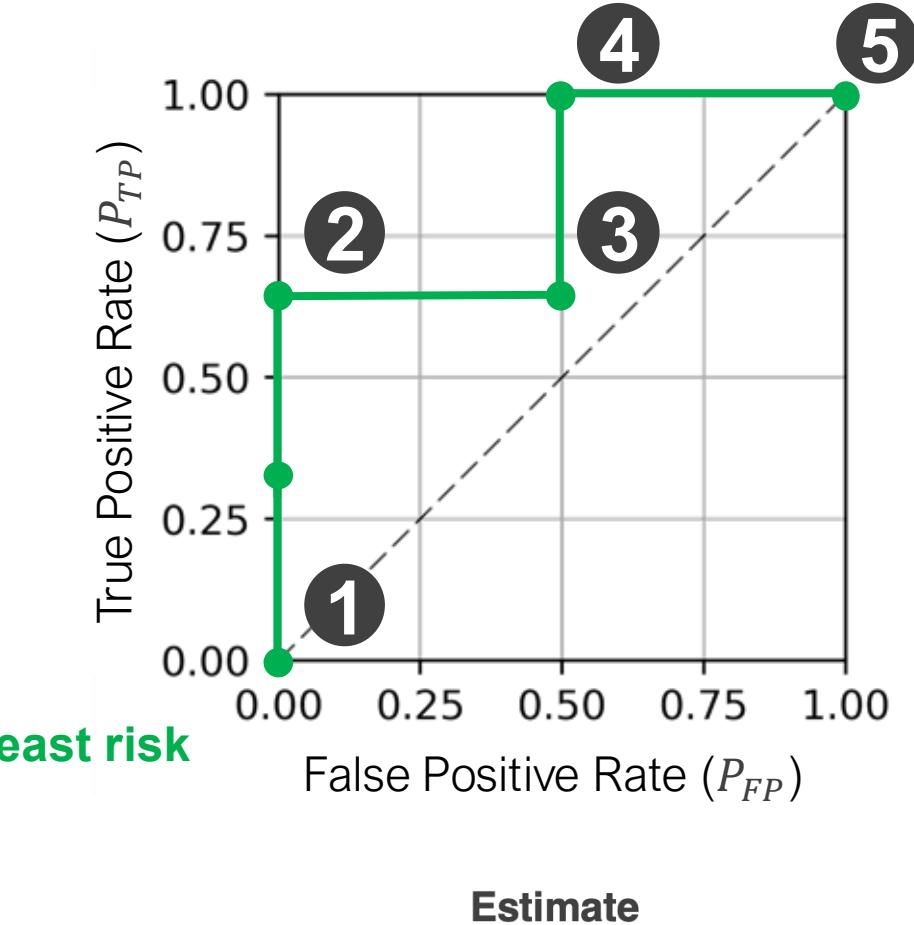
Choose where to operate

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

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

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

Truth

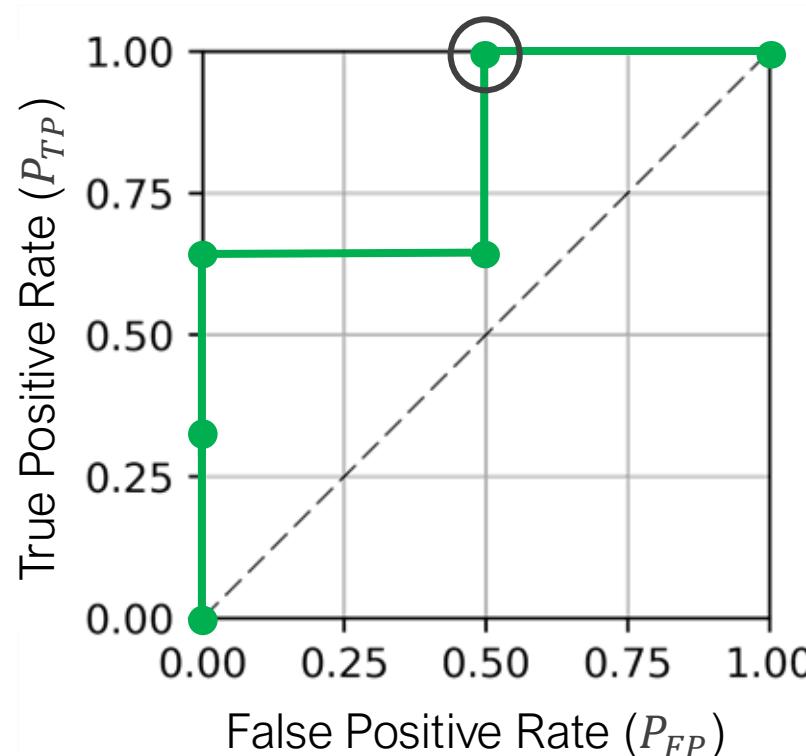


		Class 1	Class 0
		True Positive $\lambda_{11} = 0$	False negative $\lambda_{01} = 100$
		False Positive $\lambda_{10} = 1$	True Negative $\lambda_{00} = 0$
Class 1			
Class 0			

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
	Class 0	FP 25	TN 25

[50] [50]

Rates / probabilities

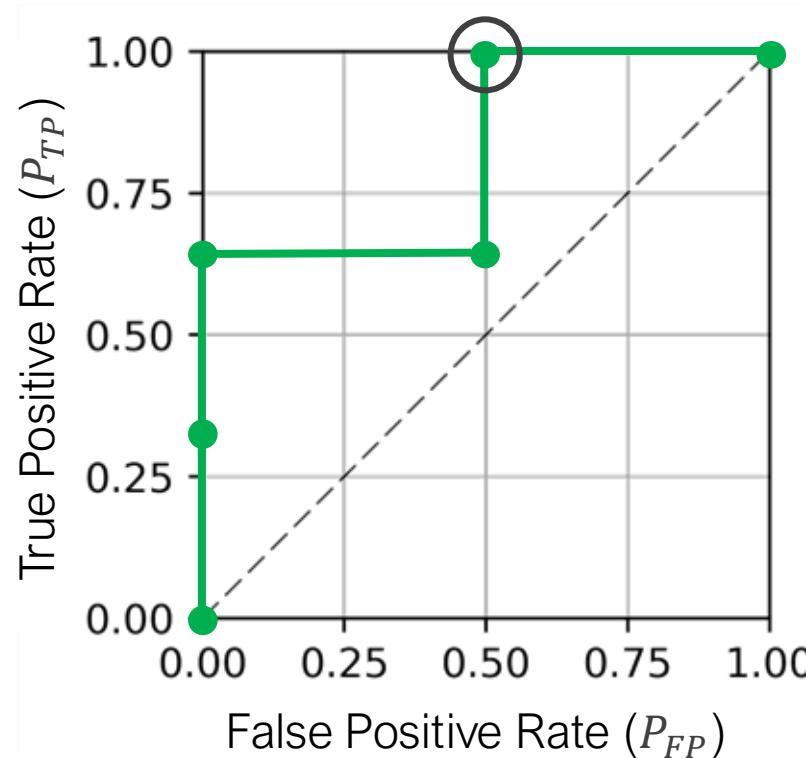
		Predicted Class	
		Class 1	Class 0
True Class	Class 1	TPR 1.0	FNR 0
	Class 0	FPR 0.5	TNR 0.5

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

[5]

[50]

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

Rates / probabilities

		Predicted Class	
		Class 1	Class 0
True Class	Class 1	TPR 1.0	FNR 0
	Class 0	FPR 0.5	TNR 0.5

[5]

[50]

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

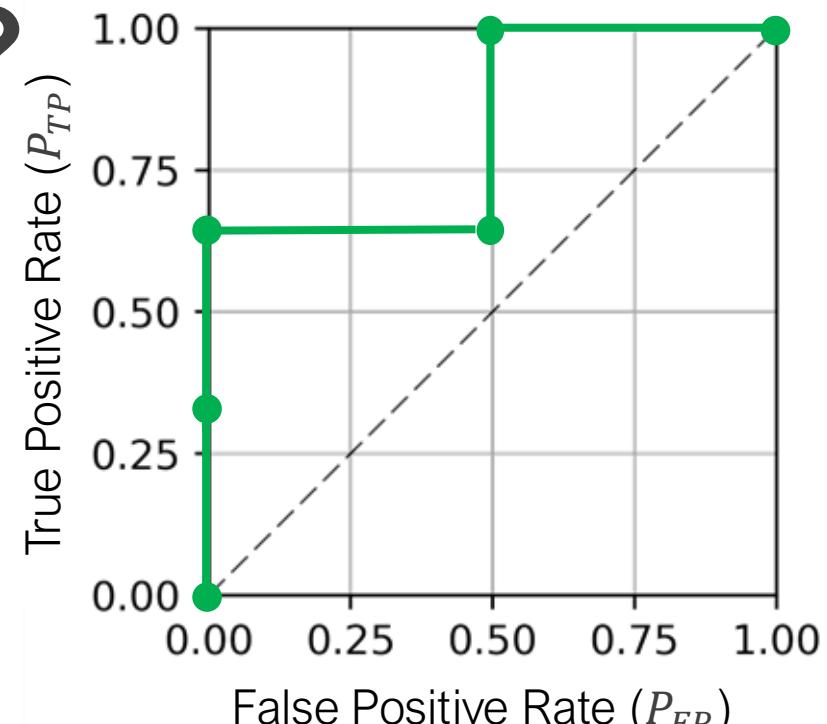
ROC curves are not sensitive to class imbalances – TPR and FPR are class-conditional

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

Class prevalence also needs to be factored in!



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

Loss if prediction is class i when truth is class j

Choose where to operate

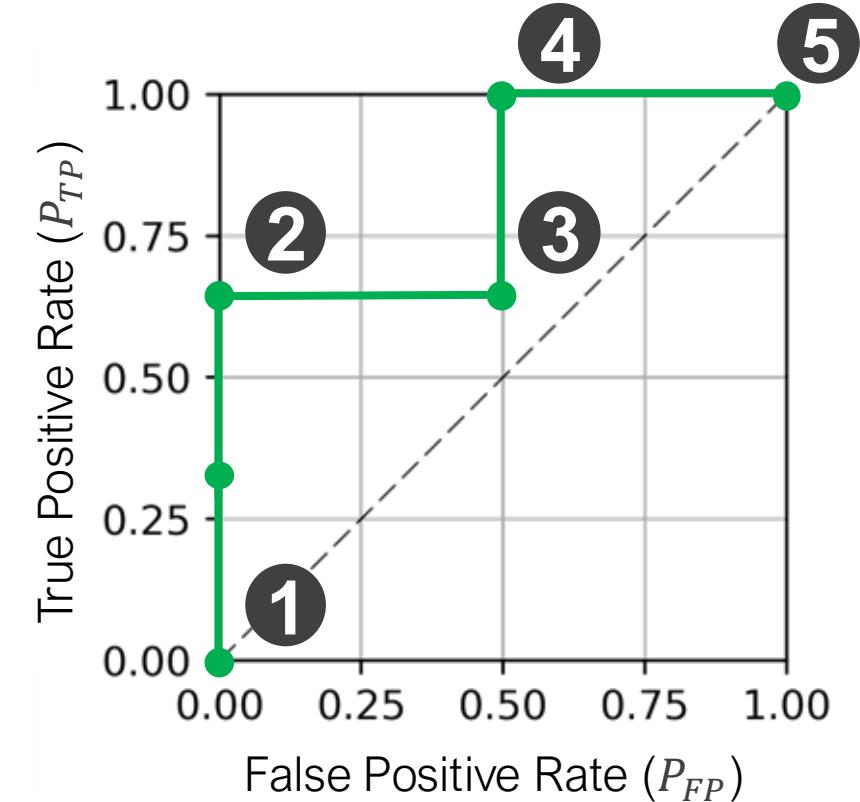
Action: select threshold k	Probability of false positive P_{FP}	Probability of false negative $P_{FN} = (1 - P_{TP})$	Risk $R(\tau_k)$
1			
2			
3			
4			
5			

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

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

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

Truth



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

Estimate

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

Choose where to operate

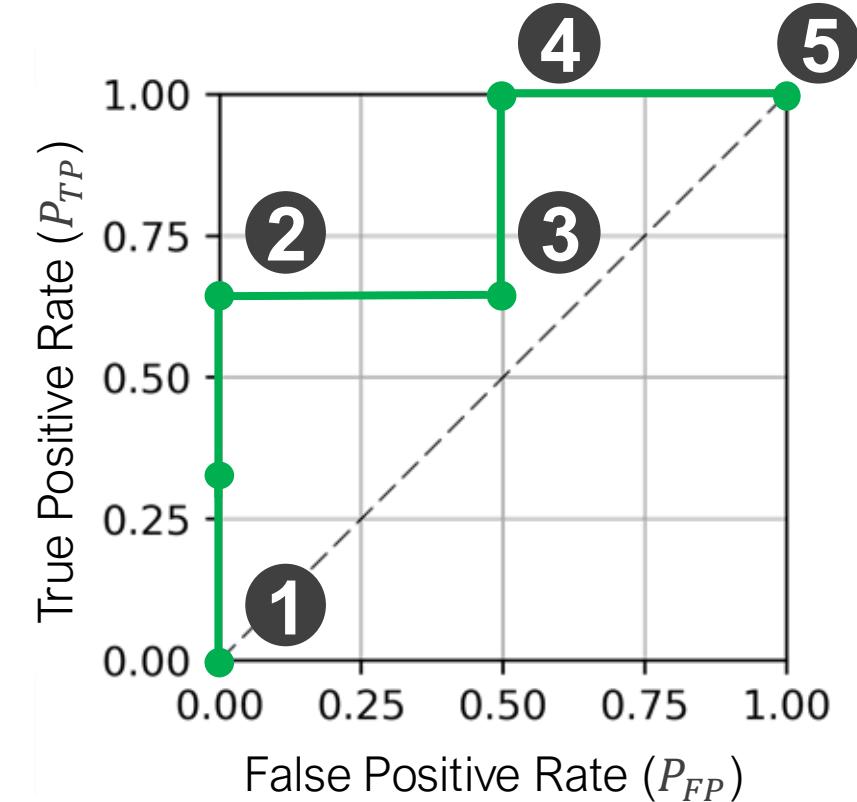
Action: select threshold k	Probability of false positive P_{FP}	Probability of false negative $P_{FN} = (1 - P_{TP})$	Risk $R(\tau_k)$
1	0	1	
2	0	0.33	
3	0.5	0.33	
4	0.5	0	
5	1	0	

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

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

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

Truth



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

Estimate

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

Choose where to operate

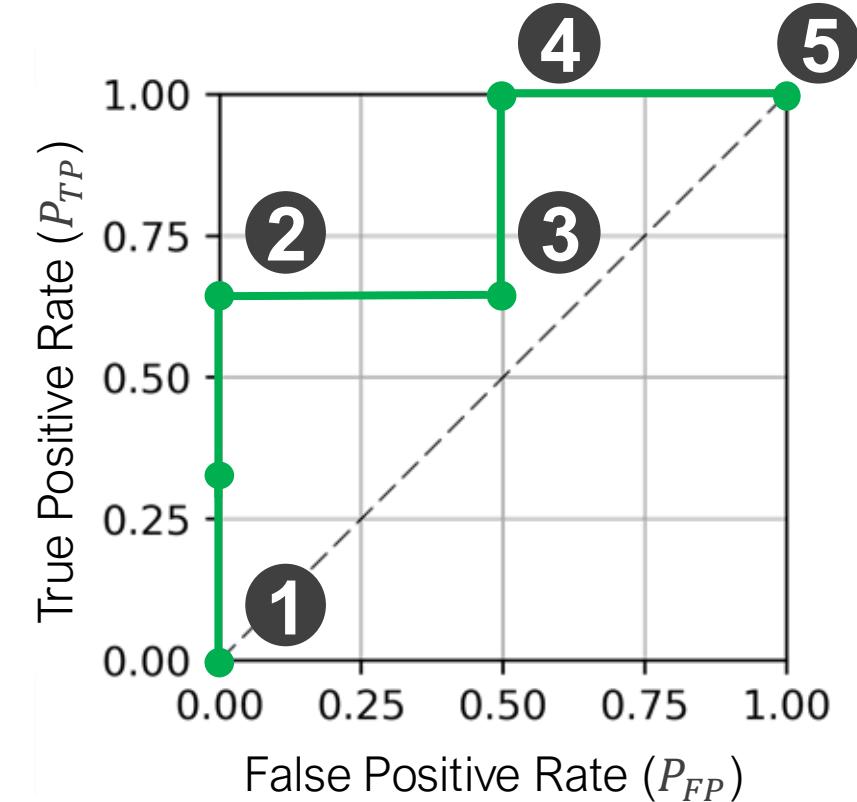
Action: select threshold k	Probability of false positive P_{FP}	Probability of false negative $P_{FN} = (1 - P_{TP})$	Risk $R(\tau_k)$
1	0	1	1
2	0	0.33	
3	0.5	0.33	
4	0.5	0	
5	1	0	

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

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

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

Truth



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

Estimate

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

Choose where to operate

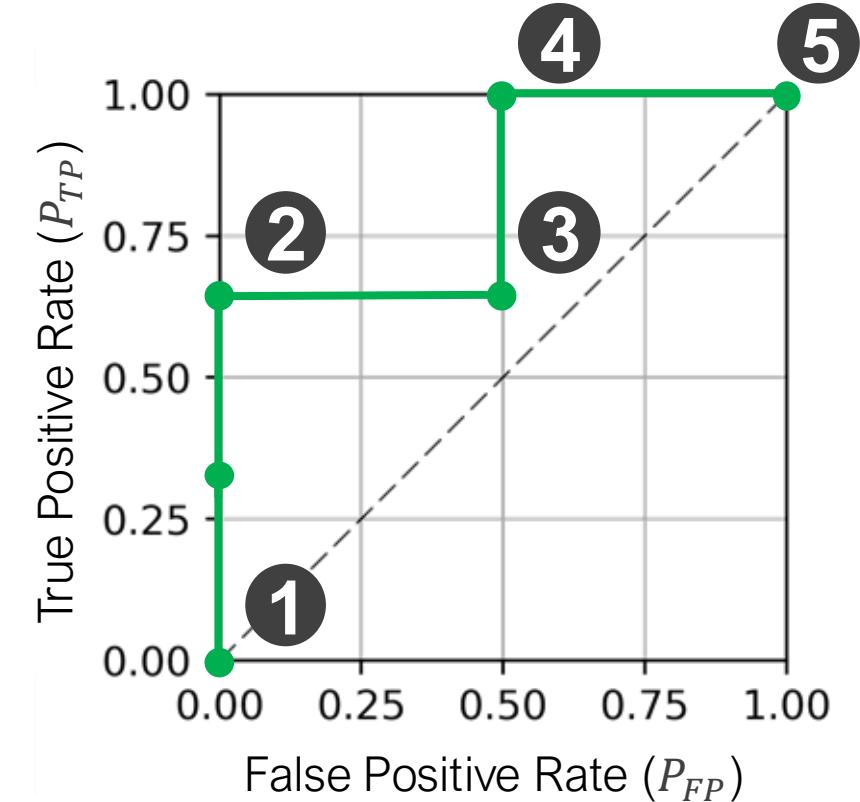
Action: select threshold k	Probability of false positive P_{FP}	Probability of false negative $P_{FN} = (1 - P_{TP})$	Risk $R(\tau_k)$
1	0	1	1
2	0	0.33	0.33
3	0.5	0.33	
4	0.5	0	
5	1	0	

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

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

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

Truth



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

Estimate

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

Choose where to operate

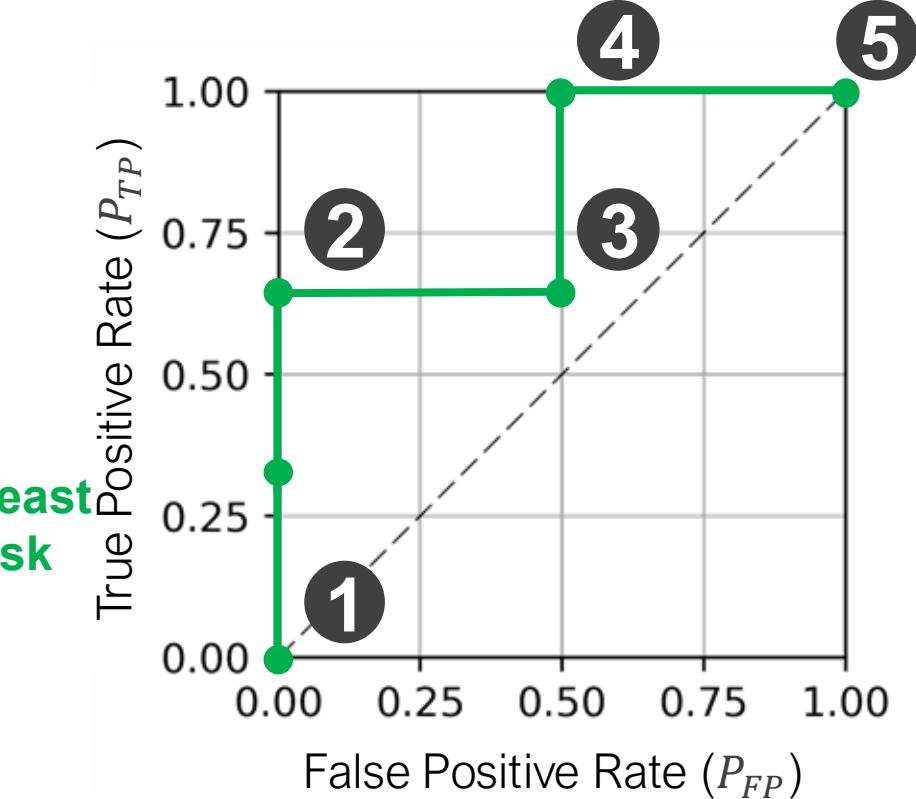
Action: select threshold k	Probability of false positive P_{FP}	Probability of false negative $P_{FN} = (1 - P_{TP})$	Risk $R(\tau_k)$
1	0	1	1
2	0	0.33	0.33
3	0.5	0.33	0.83
4	0.5	0	0.50
5	1	0	0.99

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

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

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

Truth



$$P(Y = 0) \approx 0.99$$

$$P(Y = 1) \approx 0.01$$

Estimate

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

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