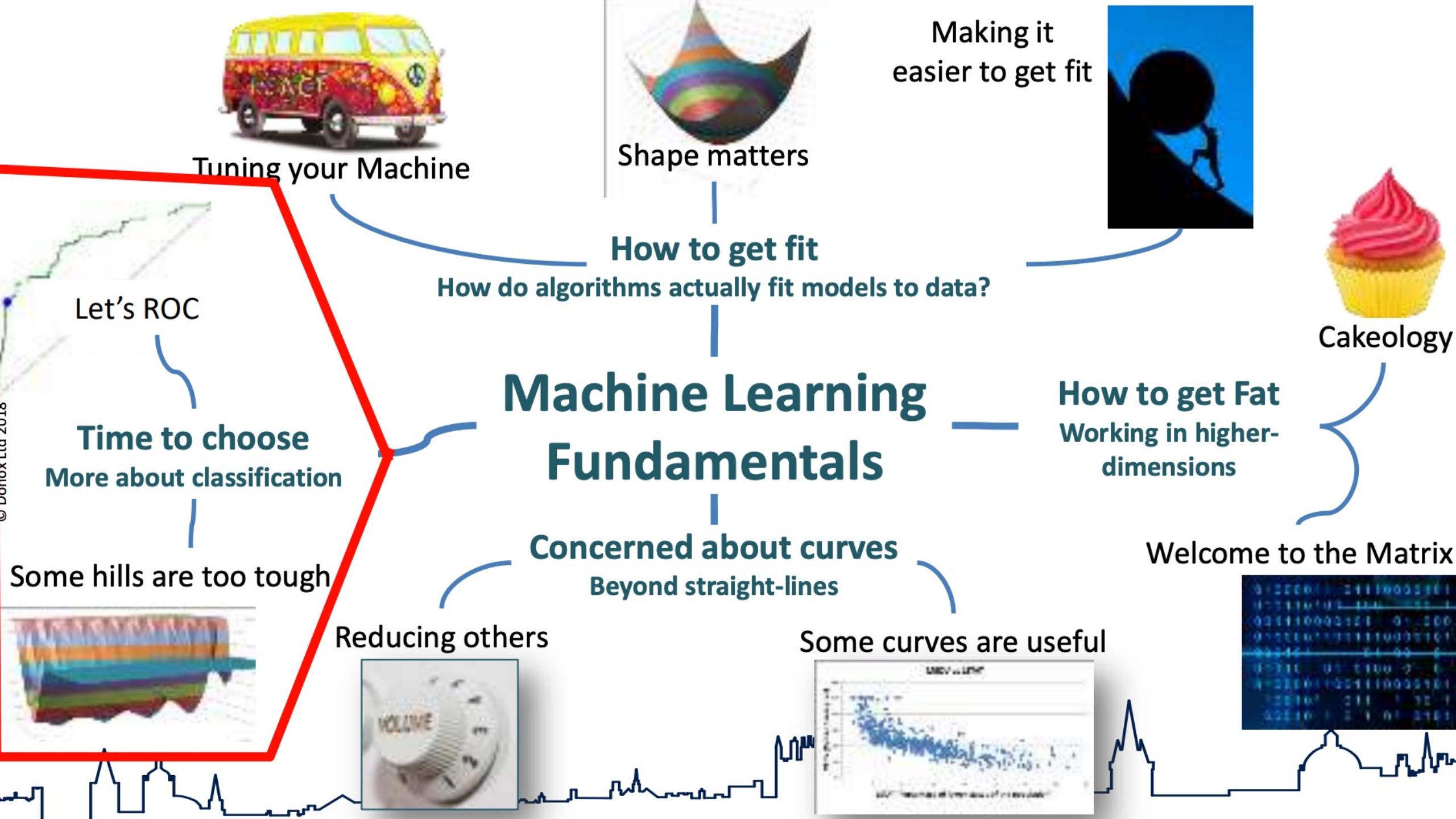


# Classification and model quality

---

Elizabeth Savochkina | 12<sup>th</sup> June





# When Models go Bad



- In 2018 the American Civil Liberties Union (ACLU) used Amazon's Rekognition facial recognition technology to compare 25,000 pictures of criminals to those members of US Congress ..
- And came up with 28 matches!



Source: <https://www.cnet.com/news/privacy/amazon-facial-recognition-thinks-28-congressmen-look-like-known-criminals-at-default-settings/>

# Predicting medical conditions

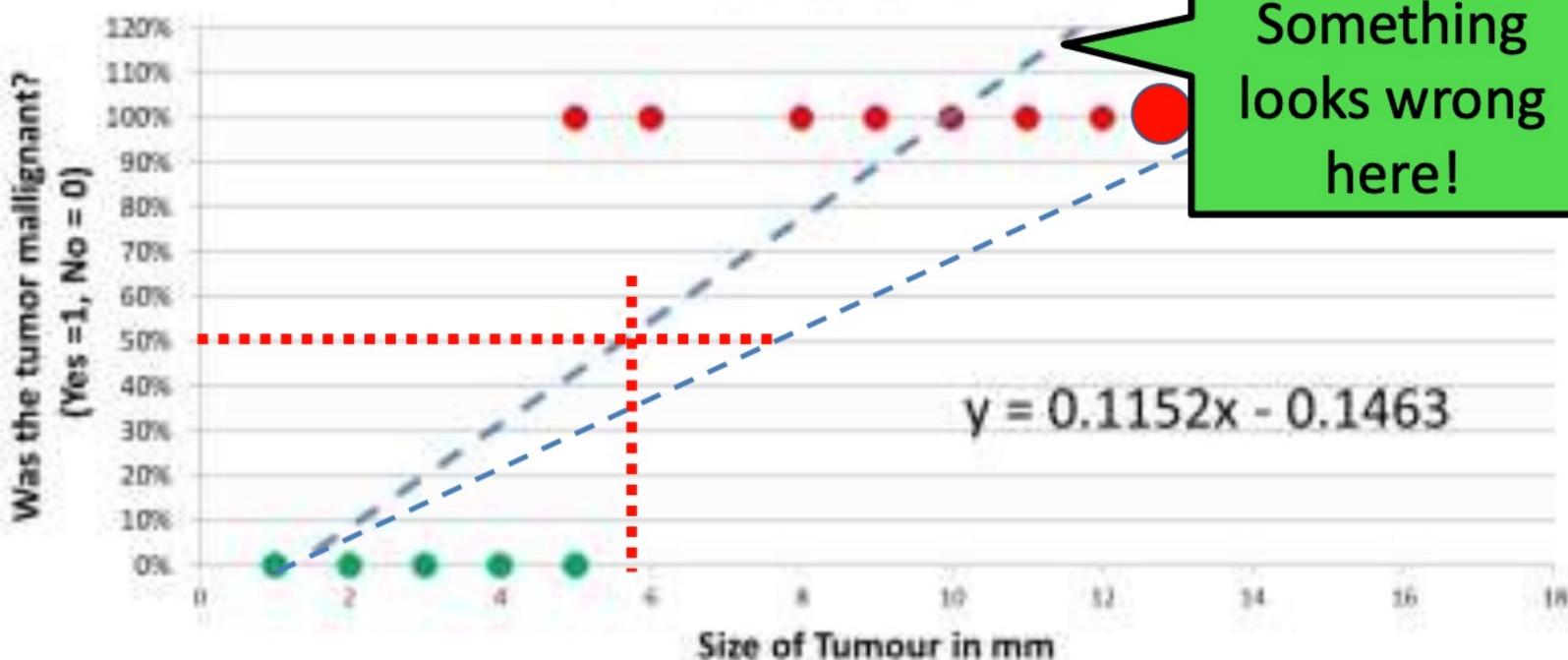
---

Consider the problem of predicting the probability of a tumour being malignant based on its size



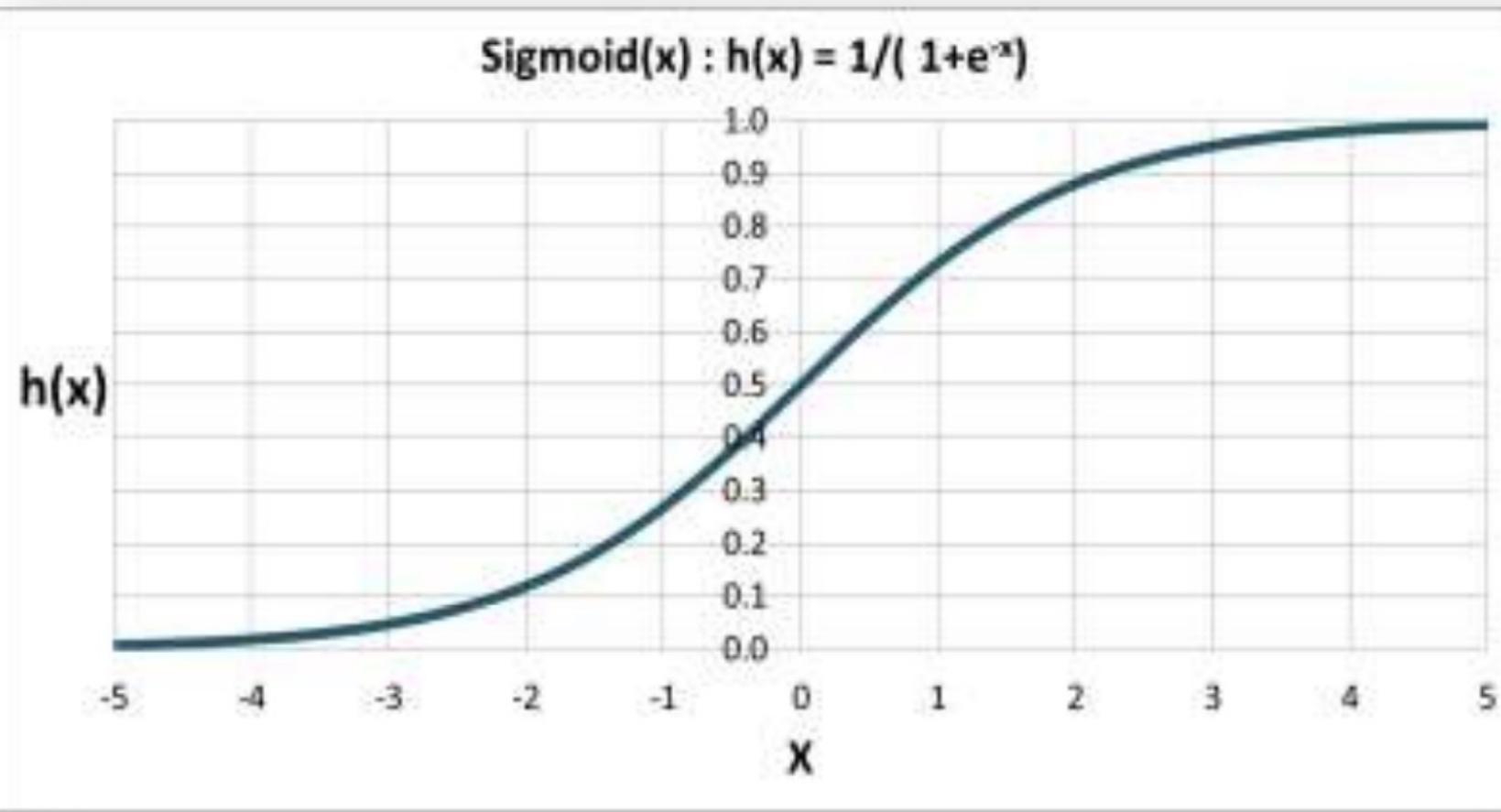
# Collect and review historical data

Relationship between size and malignancy for tumours based on historical data



- Here we have some historical data showing the relationship between 'Tumour size' and malignancy
- .. So let's just do a linear regression to make a prediction!

# An ‘S’ shaped (sigmoid) curve would be better



A sigmoid curve seems to be a better shape for model ..

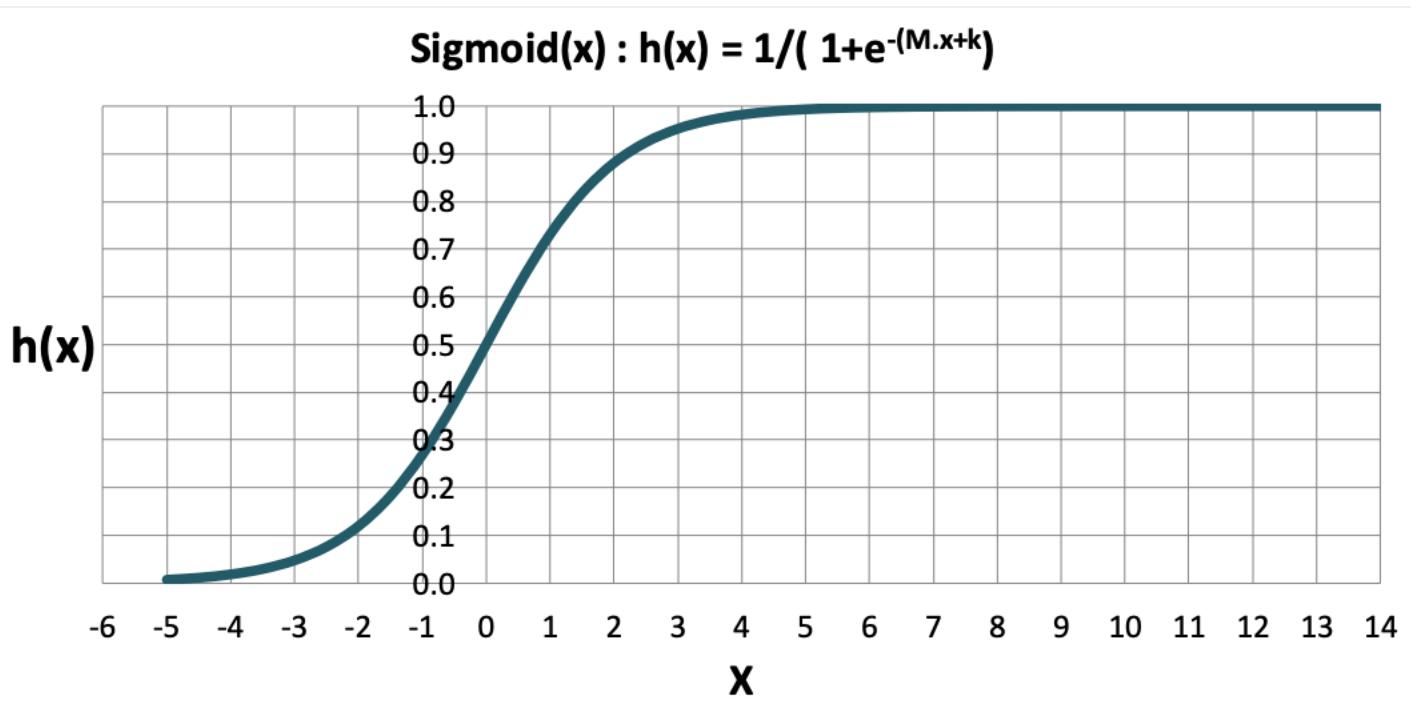
$$h(x) = \frac{1}{1 + e^{-x}}$$

‘h’ for hypothesis



# We need to modify its shape to fit the data points

k	M
0	1



$$h(x) = \frac{1}{1 + e^{-x}}$$



$$h(x) = \frac{1}{1 + e^{-(M.x+k)}}$$



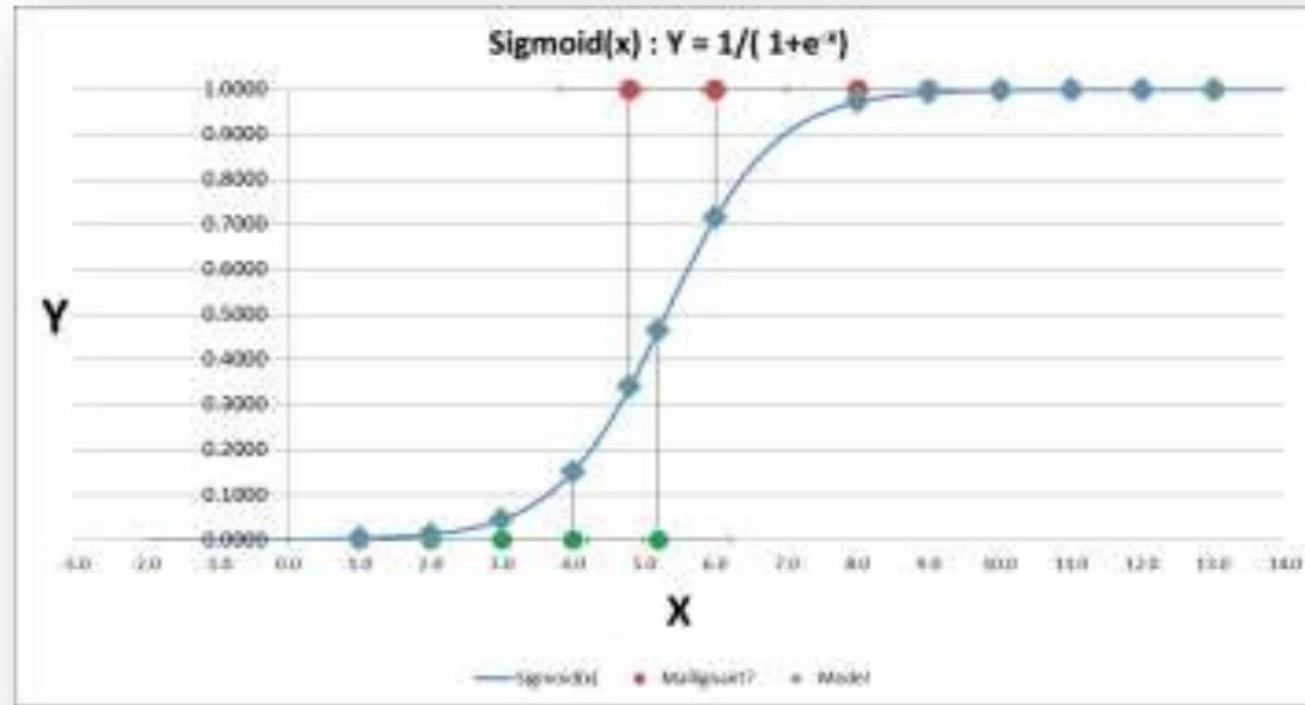
# We need a measurement to optimise a model ..

## 1 The Model



$$h(x) = \frac{1}{1 + e^{-(M \cdot x + k)}}$$

## 2 How well the model matches the data

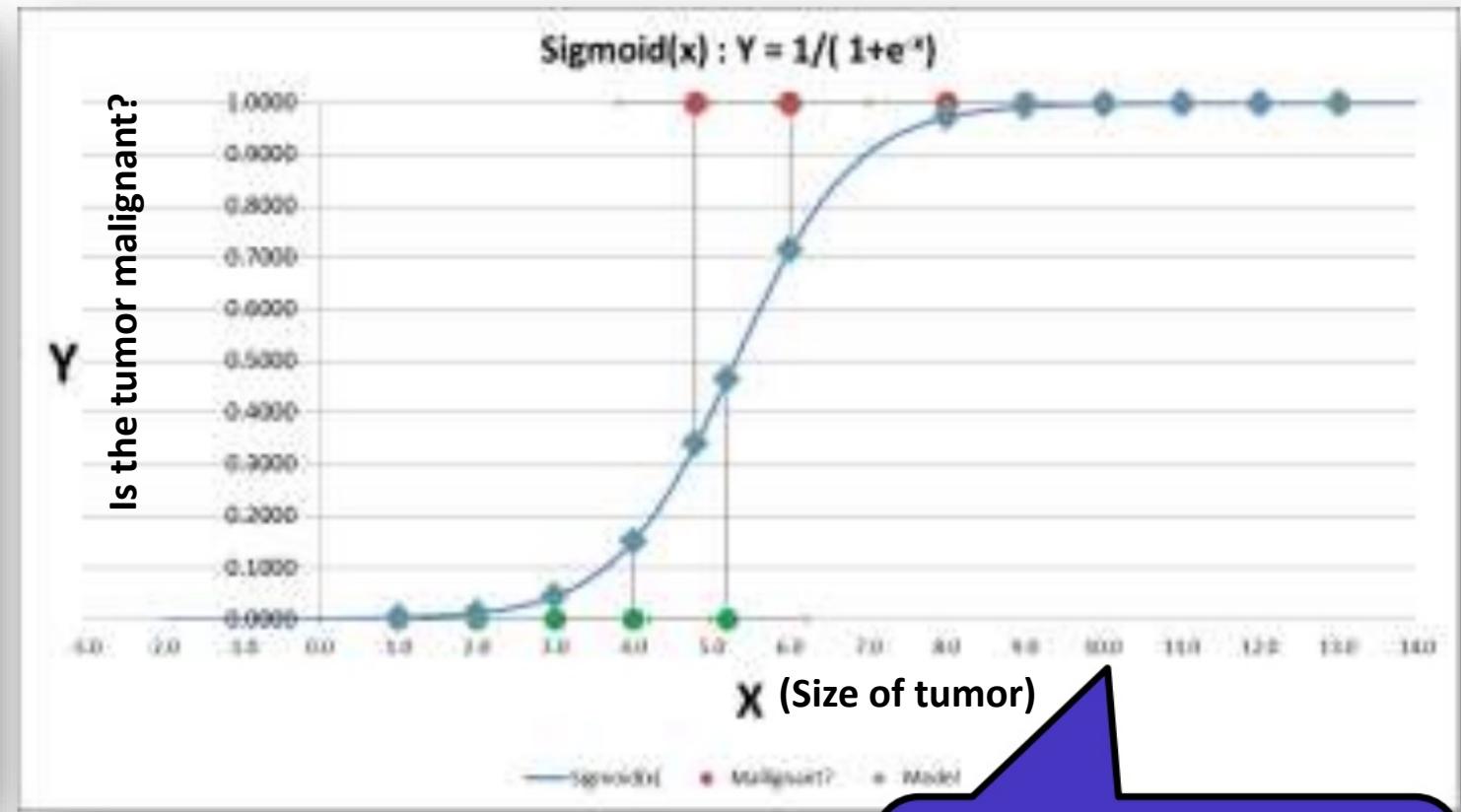


# Fitting the model by minimizing the mean square error

Size of cancer cell (mm)	Malignant?	Malignant?
1	No	0%
2	No	0%
3	No	0%
4	No	0%
4.8	Yes	100%
6	Yes	100%
5.2	No	0%
8	Yes	100%
9	Yes	100%
10	Yes	100%
11	Yes	100%
12	Yes	100%
13	Yes	100%

Model	Sq Error
0.00	0.0000
0.00	0.0000
0.01	0.0001
0.02	0.0004
0.05	0.9081
0.15	0.7280
0.07	0.0049
0.58	0.1770
0.80	0.0417
0.92	0.0069
0.97	0.0010
0.99	0.0001
1.00	0.0000

**1.8681**



Threshold (mm) that defines the person has cancer = 4.7mm tumor size

- anything above the threshold should predict – yes (100%-1), as malignant
- A new observation at 5.2mm is predicted as NOT malignant – misprediction due to a wrong loss function!

Not a good method!  
See next slide

# Gradient descent on mean square error ..

However, we have  
an issue!

We can't tune the model by minimising the mean square error

Because the parameter space is not bowl-shaped

## (Non-convex surface)



## Mean Squared Error Loss

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

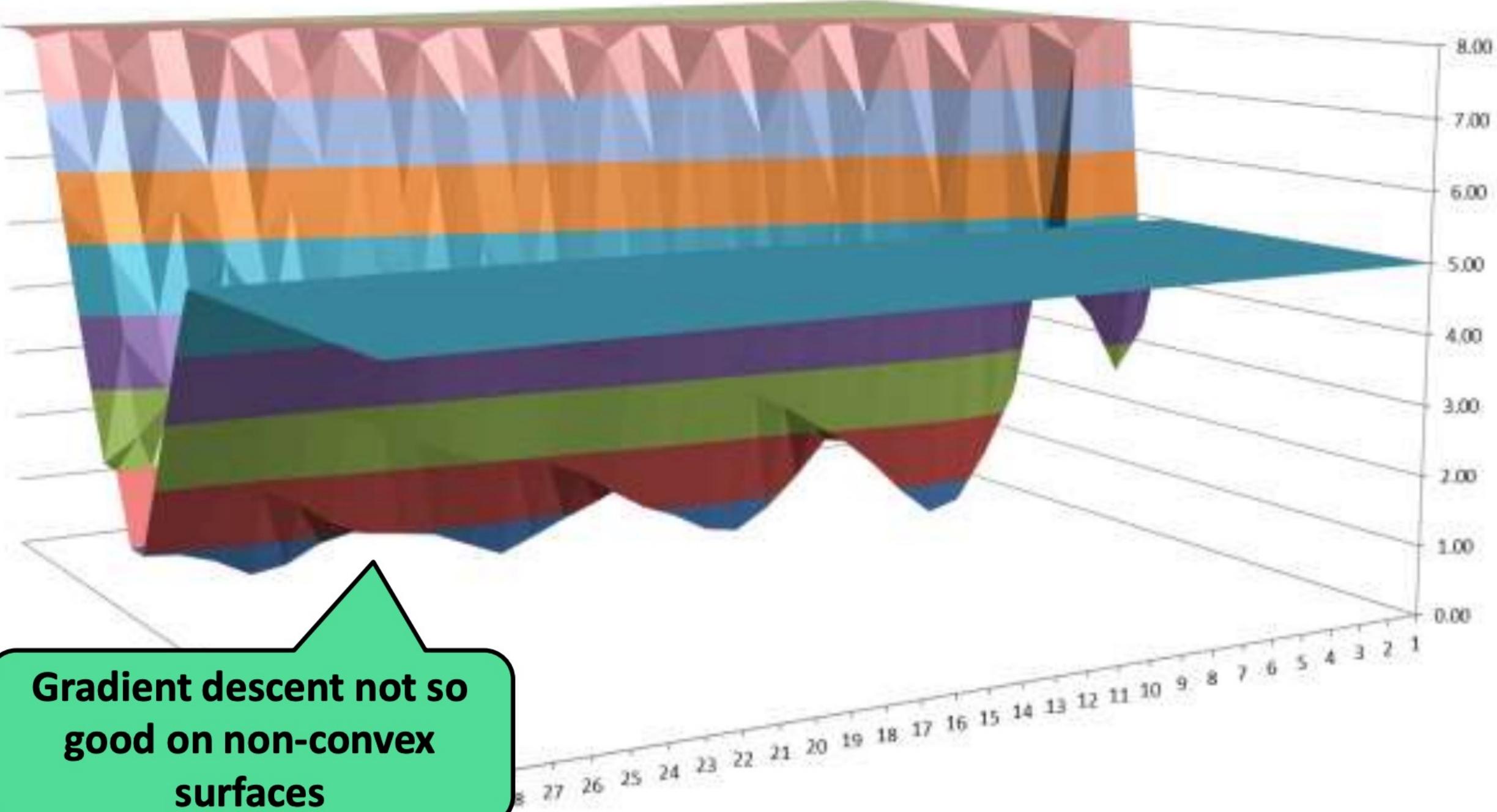
If we say:

Actual value = 1, predicted = 0

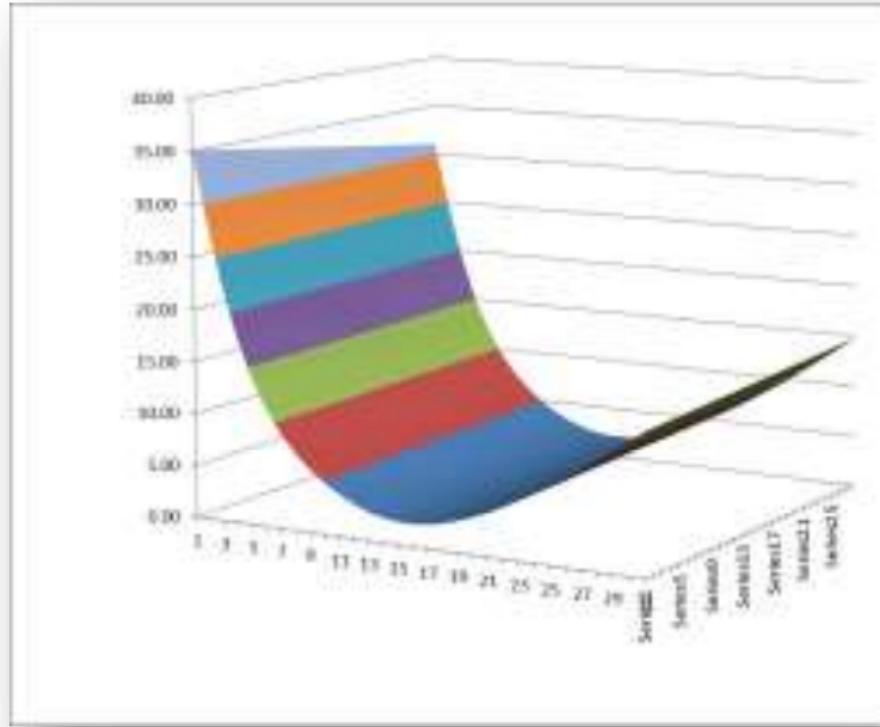
$$\text{MSE} = (1 - 0)^2 = 1$$

So, the real class is = 1 but the prediction is 0.

**MSE does not strongly penalize misclassifications** even for the perfect mismatch!



# We need an alternative to mean square error ..



$$Cost = \begin{cases} -\log(h(x)), & \text{if } y = 1, \\ -\log(1 - h(x)), & \text{if } y = 0 \end{cases}$$

## Definition of natural logarithm

When

$$e^y = x$$

Then base e logarithm of x is

$$\ln(x) = \log_e(x) = y$$

The **e constant** or Euler's number is:

$$e \approx 2.71828183$$

### Ln of 0

The natural logarithm of zero is undefined:

$\ln(0)$  is undefined

The limit near 0 of the natural logarithm of x, when x approaches zero, is minus infinity:

$$\lim_{x \rightarrow 0^+} \ln(x) = -\infty$$

$$\text{LogLoss} = \frac{-1}{N} \sum_{i=1}^N \sum_{j=1}^M x_{ij} * \log(p_{ij})$$

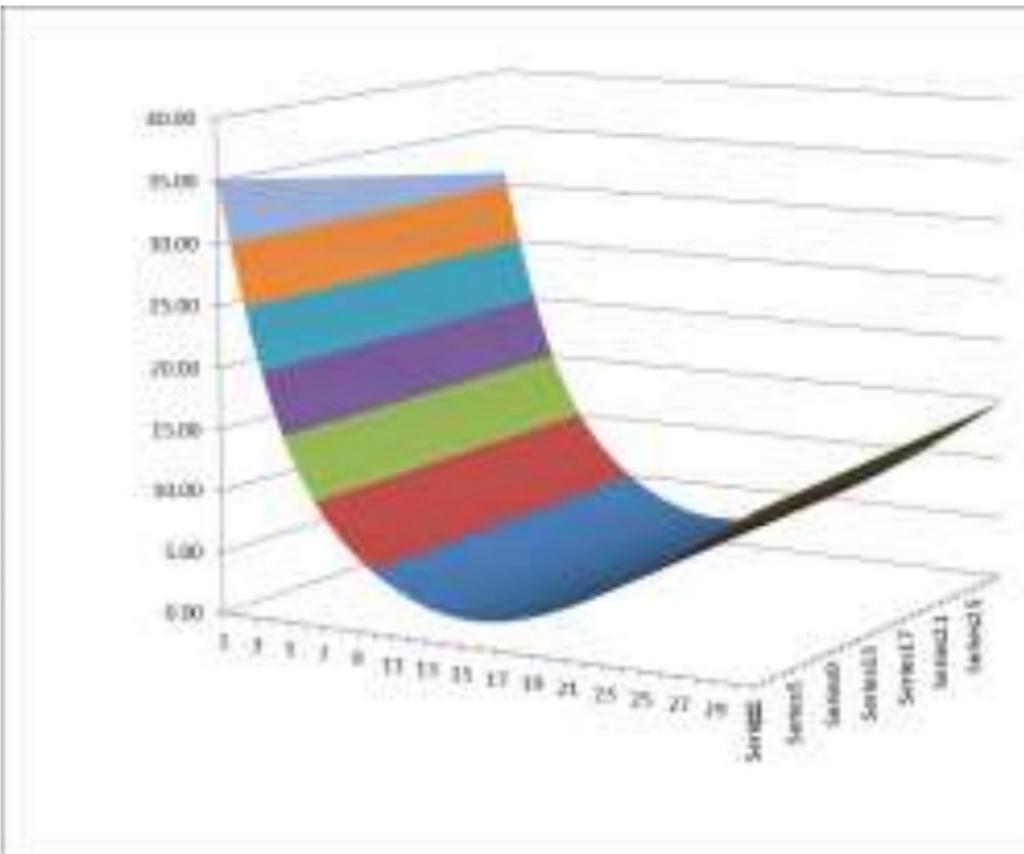
If we say:

Actual value = 1, predicted = 0

**LogLoss = -(1 \* log(0) + 0 \* log(1)) = tends to infinity !!**

**LogLoss strongly penalizes misclassifications where loss tends to infinity!**

# We need an alternative to mean square error ..

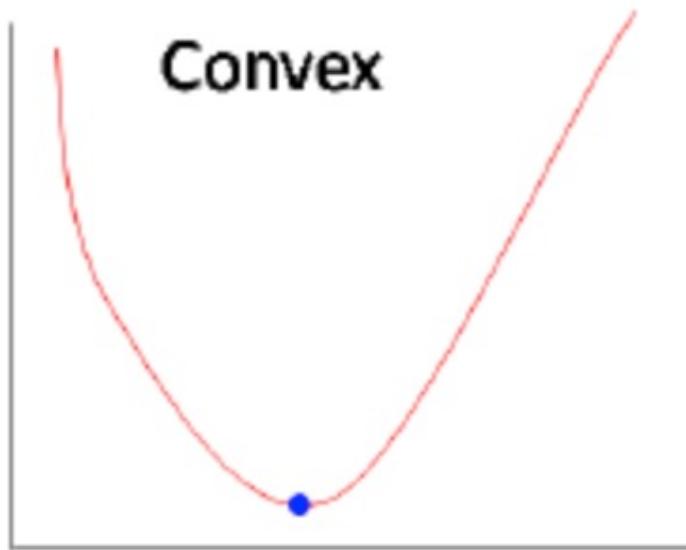


	k →																											
	-10.8	-10.8	-10.8	-10.7	-10.7	-10.7	-10.7	-10.6	-10.6	-10.6	-10.6	-10.5	-10.5	-10.5	-10.5	-10.4	-10.4	-10.4	-10.4	-10.3	-10.3	-10.3	-10.3					
0.70	35.08	34.93	34.77	34.62	34.47	34.31	34.16	34.01	33.86	33.70	33.55	33.40	33.25	33.10	32.94	32.79	32.64	32.49	32.34	32.19	32.04	31.88	31.73	31.58	31.43	31.28	31.13	30.98
0.80	28.37	28.22	28.08	27.94	27.80	27.66	27.51	27.37	27.23	27.09	26.95	26.81	26.67	26.53	26.39	26.25	26.11	25.98	25.84	25.70	25.56	25.42	25.29	25.15	25.01	24.88	24.74	24.61
0.90	22.51	22.38	22.26	22.14	22.01	21.89	21.77	21.64	21.52	21.40	21.28	21.15	21.03	20.91	20.79	20.67	20.55	20.43	20.31	20.20	20.08	19.96	19.84	19.73	19.61	19.49	19.38	19.26
1.00	17.77	17.66	17.56	17.45	17.35	17.24	17.14	17.04	16.94	16.83	16.73	16.63	16.53	16.43	16.33	16.23	16.13	16.03	15.93	15.84	15.74	15.64	15.54	15.45	15.35	15.25	15.16	15.06
1.10	14.07	13.98	13.90	13.81	13.73	13.64	13.56	13.47	13.39	13.30	13.22	13.14	13.05	12.97	12.89	12.81	12.73	12.64	12.56	12.48	12.40	12.32	12.24	12.16	12.09	12.01	11.93	11.85
1.20	11.23	11.16	11.09	11.02	10.95	10.88	10.81	10.74	10.67	10.60	10.53	10.46	10.39	10.33	10.26	10.19	10.13	10.06	9.99	9.93	9.86	9.80	9.73	9.67	9.60	9.54	9.47	9.41
1.30	9.04	8.98	8.92	8.87	8.81	8.75	8.69	8.63	8.58	8.52	8.46	8.41	8.35	8.30	8.24	8.19	8.13	8.08	8.02	7.97	7.91	7.86	7.81	7.75	7.70	7.65	7.59	7.54
1.40	7.34	7.29	7.24	7.19	7.14	7.10	7.05	7.00	6.95	6.91	6.86	6.81	6.76	6.72	6.67	6.63	6.58	6.53	6.49	6.44	6.40	6.35	6.31	6.26	6.22	6.18	6.13	6.09
1.50	5.99	5.94	5.90	5.86	5.82	5.78	5.74	5.70	5.66	5.62	5.58	5.54	5.50	5.46	5.42	5.38	5.34	5.30	5.26	5.23	5.19	5.15	5.11	5.08	5.04	5.00	4.96	4.93
1.60	4.88	4.85	4.81	4.78	4.74	4.71	4.67	4.64	4.60	4.57	4.53	4.50	4.47	4.43	4.40	4.37	4.33	4.30	4.27	4.24	4.20	4.17	4.14	4.11	4.08	4.05	4.02	3.99
1.70	3.97	3.94	3.91	3.88	3.85	3.83	3.80	3.77	3.74	3.71	3.68	3.65	3.63	3.60	3.57	3.54	3.52	3.49	3.46	3.44	3.41	3.39	3.36	3.34	3.31	3.29	3.26	3.24
1.80	3.24	3.22	3.19	3.17	3.15	3.12	3.10	3.08	3.05	3.03	3.01	2.99	2.97	2.95	2.92	2.90	2.88	2.86	2.84	2.82	2.80	2.78	2.77	2.75	2.73	2.71	2.69	2.67
1.90	2.69	2.67	2.65	2.63	2.62	2.60	2.58	2.57	2.55	2.54	2.52	2.51	2.49	2.48	2.46	2.45	2.44	2.42	2.41	2.40	2.38	2.37	2.36	2.35	2.34	2.33	2.31	2.30
2.00	2.31	2.30	2.29	2.28	2.27	2.26	2.25	2.25	2.24	2.23	2.22	2.21	2.20	2.20	2.19	2.18	2.18	2.17	2.16	2.16	2.15	2.15	2.14	2.14	2.13	2.13	2.12	
2.10	2.13	2.12	2.12	2.12	2.11	2.11	2.11	2.11	2.11	2.11	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.11	2.11	2.11	2.12	2.12	
2.20	2.12	2.12	2.12	2.13	2.13	2.13	2.14	2.14	2.15	2.15	2.16	2.16	2.17	2.18	2.18	2.19	2.20	2.20	2.21	2.22	2.23	2.24	2.24	2.25	2.26	2.27	2.28	2.29
2.30	2.27	2.28	2.29	2.30	2.31	2.32	2.33	2.34	2.35	2.36	2.37	2.39	2.40	2.41	2.42	2.45	2.46	2.48	2.49	2.50	2.52	2.53	2.56	2.58	2.59	2.61		
2.40	2.57	2.58	2.60	2.61	2.63	2.65	2.66	2.68	2.69	2.71	2.73	2.75	2.76	2.78	2.80	2.82	2.84	2.86	2.87	2.89	2.91	2.93	2.95	2.97	2.99	3.01	3.03	3.06
2.50	2.99	3.01	3.03	3.06	3.08	3.10	3.12	3.14	3.16	3.18	3.21	3.23	3.25	3.27	3.30	3.32	3.37	3.39	3.41	3.44	3.46	3.49	3.51	3.54	3.56	3.59	3.61	
2.60	3.53	3.55	3.58	3.60	3.63	3.65	3.68	3.70	3.73	3.76	3.78	3.81	3.84	3.86	3.89	3.92	3.97	4.00	4.03	4.06	4.09	4.11	4.14	4.17	4.20	4.23	4.26	
2.70	4.16	4.18	4.21	4.24	4.27	4.30	4.33	4.36	4.39	4.42	4.45	4.48	4.51	4.54	4.57	4.60	4.66	4.70	4.73	4.76	4.79	4.82	4.85	4.89	4.92	4.95	4.99	
2.80	4.86	4.89	4.92	4.96	4.99	5.02	5.05	5.09	5.12	5.15	5.19	5.22	5.25	5.29	5.32	5.36	5.40	5.45	5.50	5.53	5.57	5.60	5.64	5.67	5.71	5.74	5.78	
2.90	5.63	5.67	5.70	5.74	5.77	5.81	5.84	5.88	5.92	5.95	5.99	6.03	6.06	6.10	6.14	6.17	6.21	6.23	6.32	6.36	6.40	6.44	6.48	6.51	6.55	6.59	6.63	
3.00	6.46	6.50	6.54	6.57	6.61	6.65	6.69	6.73	6.77	6.81	6.84	6.88	6.92	6.96	7.00	7.04	7.08	7.20	7.24	7.28	7.32	7.36	7.40	7.44	7.49	7.53		
3.10	7.34	7.38	7.42	7.46	7.50	7.54	7.58	7.62	7.66	7.70	7.74	7.79	7.83	7.87	7.91	7.95	8.00	8.12	8.16	8.21	8.25	8.29	8.34	8.38	8.42	8.47		
3.20	8.26	8.30	8.34	8.38	8.43	8.47	8.51	8.56	8.60	8.64	8.68	8.73	8.77	8.82	8.86	8.90									9.11	9.35	9.40	9.44
3.30	9.21	9.26	9.30	9.35	9.39	9.43	9.48	9.52	9.57	9.62	9.66	9.71	9.75	9.80	9.84	9.89									10.31	10.36	10.40	10.45
3.40	10.20	10.25	10.29	10.34	10.39	10.43	10.48	10.53	10.57	10.62	10.67	10.72	10.76	10.81	10.86	10.91									11.35	11.39	11.44	11.49
3.50	11.22	11.27	11.32	11.37	11.41	11.46	11.51	11.56	11.61	11.66	11.71	11.76	11.81	11.86	11.91	11.96									12.41	12.46	12.51	12.56
3.60	12.27	12.32	12.37	12.42	12.47	12.52	12.57	12.62	12.67	12.72	12.78	12.83	12.88	12.93	12.98	13.03									13.50	13.56	13.61	13.66
3.70	13.35	13.40	13.45	13.50	13.56	13.61	13.66	13.71	13.77	13.82	13.87	13.92	13.98	14.03	14.08	14.14									14.62	14.68	14.73	14.79

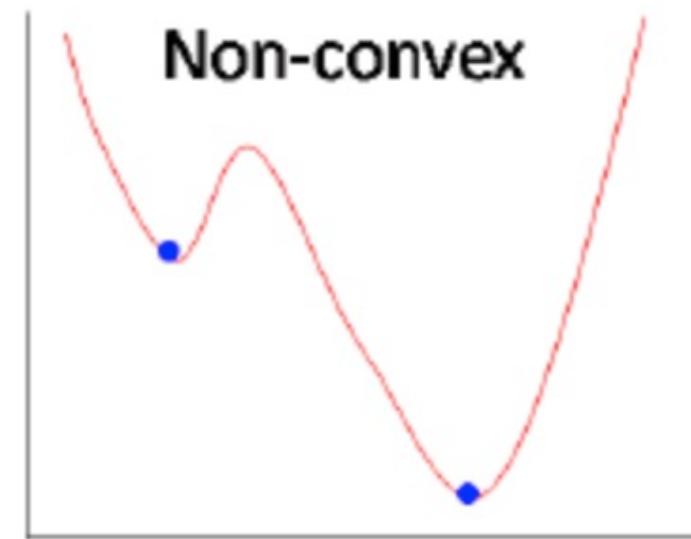
$$\begin{array}{l} M \sim 2 \\ K \sim -10 \end{array}$$



## Logarithmic loss



## MSE loss



- MSE function is non-convex for binary classification
- it is *not guaranteed* to minimize the Cost function.

# In Python .. Easier than Excel!

```
In [1]: 1 from sklearn.linear_model import LogisticRegression
```

```
In [2]: 1 x = [ [ 1. ], [ 2. ], [ 3. ], [ 4. ], [ 4.8], [ 6. ],
2           [ 5.2], [ 8. ], [ 9. ], [10. ], [11. ], [12. ], [13. ]]
3 Y = [0,0,0,0,1,1,0,1,1,1,1,1,1]
```

```
In [3]: 1 logisticRegr = LogisticRegression(solver='liblinear', C=1e9)
```

```
In [ ]: 1 logisticRegr.fit(x,Y)
```

```
In [5]: 1 print(logisticRegr.coef_)
2 print(logisticRegr.intercept_)

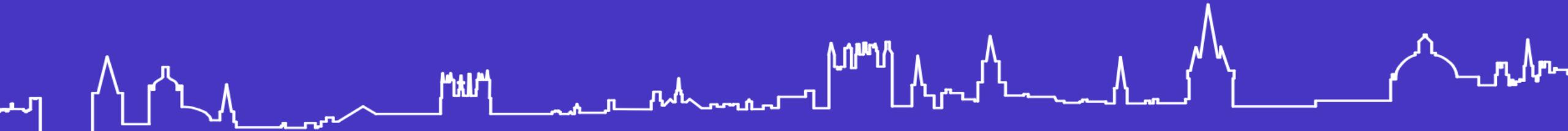
[[2.16244588]]
[-10.8314298]
```

Student task .. Replicate  
this in RapidMiner

---

# The Language of Model Quality

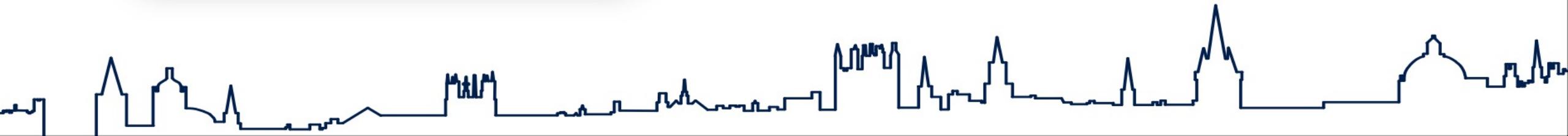
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# Recall Week 1 : Logistical Regression for Credit Analysis



		Prediction	
		No Default	Default
Reality	No Default	Computer said "They will not default". We gave them a loan. They <u>did not</u> default. <b>Good business!</b>	Computer said "They will default". We didn't give them a loan. Lost business. <b>Not good</b>
	Default	Computer said "They will not default". We gave them a loan. They <u>did</u> default. <b>Bad!</b>	Computer said "They will default". We did not give them a loan. They <u>would have</u> defaulted in reality <b>Good decision</b>



		Prediction	
		No Default	Default
Reality	No Default	Computer said "They will not default". We gave them a loan. They <u>did not</u> default. Good business!	Computer said "They will default". We didn't give them a loan. Lost business. Not good
	Default	Computer said "They will not default". We gave them a loan. They <u>did</u> default. Bad!	Computer said "They will default". We did not give them a loan. They <u>would</u> have defaulted in reality Good decision

TP - A true positive is an outcome where the model correctly predicts the positive class.

TN - A true negative is an outcome where the model correctly predicts the negative class.

FP - A false positive is an outcome where the model incorrectly predicts the positive class.

FN - A false negative is an outcome where the model incorrectly predicts the negative class.

# F<sub>1</sub>-score

---

- The F<sub>1</sub>-score is a way of combining the precision and recall of a model
- Defined as the harmonic mean of the model's precision and recall.

$$\begin{aligned}F_1 &= \frac{2}{\frac{1}{\text{recall}} \times \frac{1}{\text{precision}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \\&= \frac{\text{tp}}{\text{tp} + \frac{1}{2}(\text{fp} + \text{fn})}\end{aligned}$$



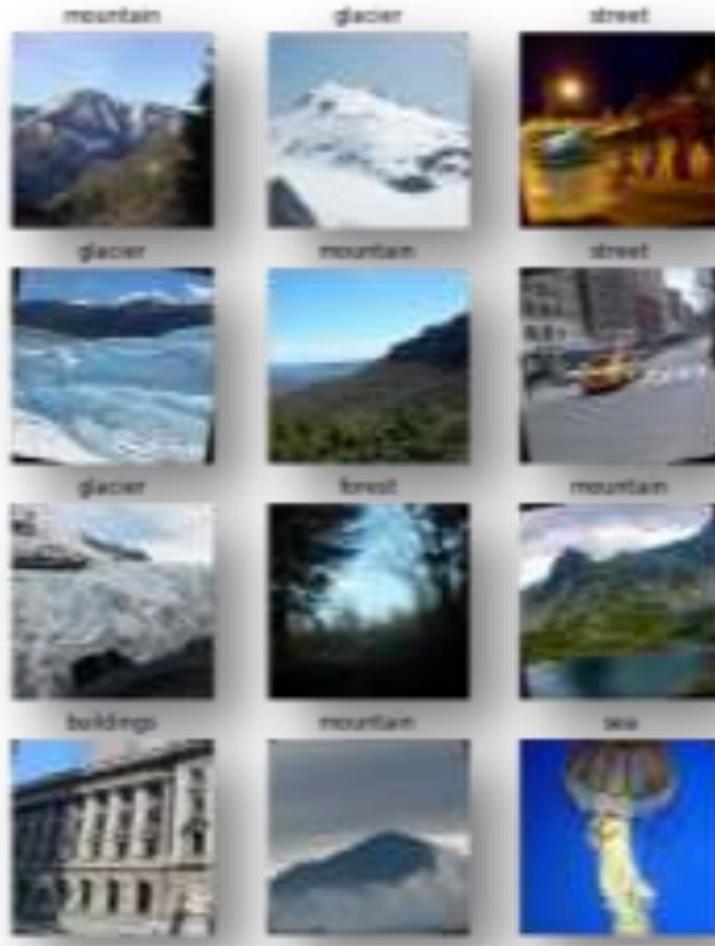
# What is a good F<sub>1</sub>-score?

---

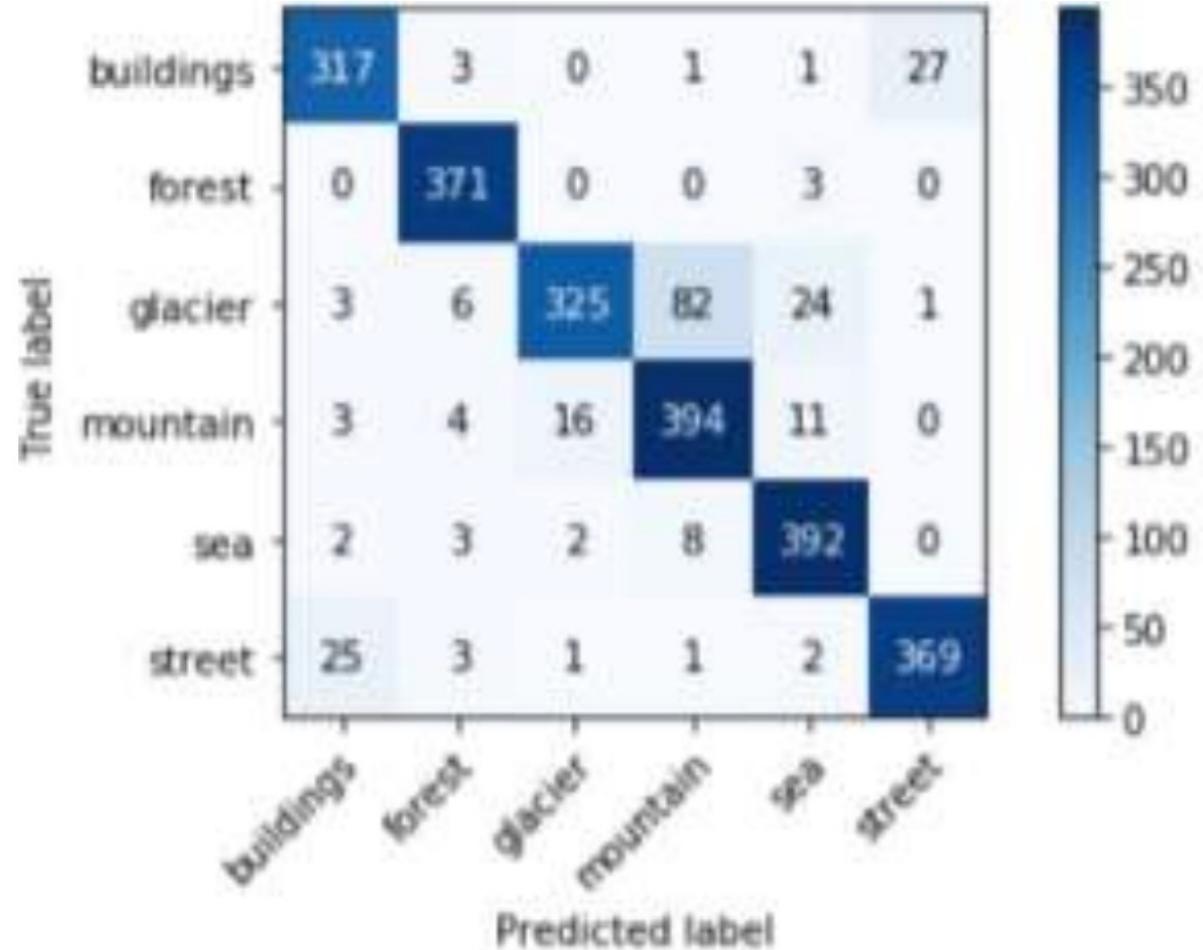
- F1 score ranges from 0 to 1
- 1 is a perfect score indicating that the model predicts each observation correctly.
- In general:
  - > 0.9 Very good
  - 0.8 - 0.9 Good
  - 0.5 - 0.8 OK
  - < 0.5 Not good



# Multi-Class Classification



Training set ~2200 images of each classification



Source: <https://medium.com/swlh/image-classification-tutorials-in-pytorch-transfer-learning-19ebc329e200>

# sklearn.metrics.classification\_report

Classification report for classifier

SVC(gamma=0.001):

	precision	recall	f1-score	support
--	-----------	--------	----------	---------

0	1.00	0.99	0.99	88
1	0.99	0.97	0.98	91
2	0.99	0.99	0.99	86
3	0.98	0.87	0.92	91
4	0.99	0.96	0.97	92
5	0.95	0.97	0.96	91
6	0.99	0.99	0.99	91
7	0.96	0.99	0.97	89
8	0.94	1.00	0.97	88
9	0.93	0.98	0.95	92

accuracy

0.97 899

Confusion matrix:

```
[87 0 0 0 1 0 0 0 0 0]  
[0 88 1 0 0 0 0 0 1 1]  
[0 0 85 1 0 0 0 0 0 0]  
[0 0 0 79 0 3 0 4 5 0]  
[0 0 0 0 88 0 0 0 0 4]  
[0 0 0 0 0 88 1 0 0 2]  
[0 1 0 0 0 0 90 0 0 0]  
[0 0 0 0 0 1 0 88 0 0]  
[0 0 0 0 0 0 0 0 88 0]  
[0 0 0 1 0 1 0 0 0 90]]
```

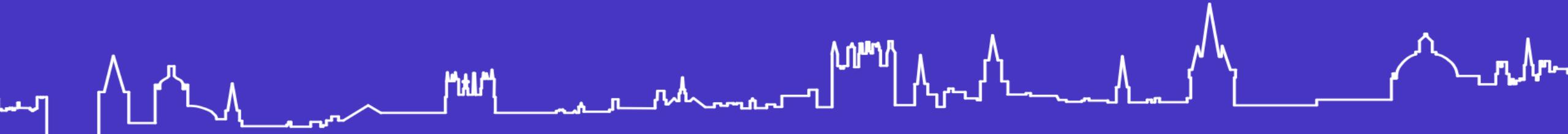
Sources: [https://scikit-learn.org/stable/auto\\_examples/classification/plot\\_digits\\_classification.html#sphx-glr-auto-examples-classification-plot-digits-classification-py](https://scikit-learn.org/stable/auto_examples/classification/plot_digits_classification.html#sphx-glr-auto-examples-classification-plot-digits-classification-py)  
[https://scikit-learn.org/stable/modules/generated/sklearn.metrics.classification\\_report.html](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.classification_report.html)



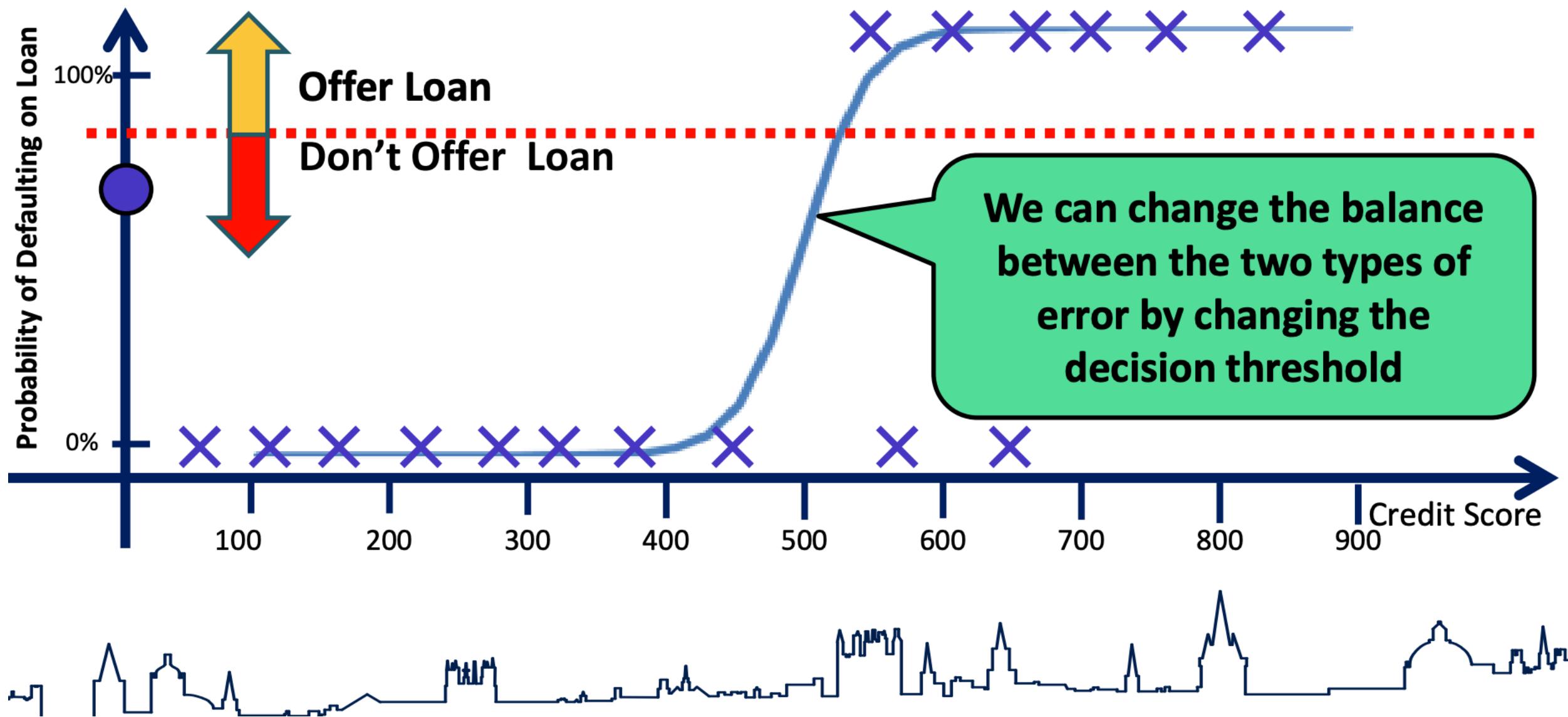
---

# Moving the decision point

---

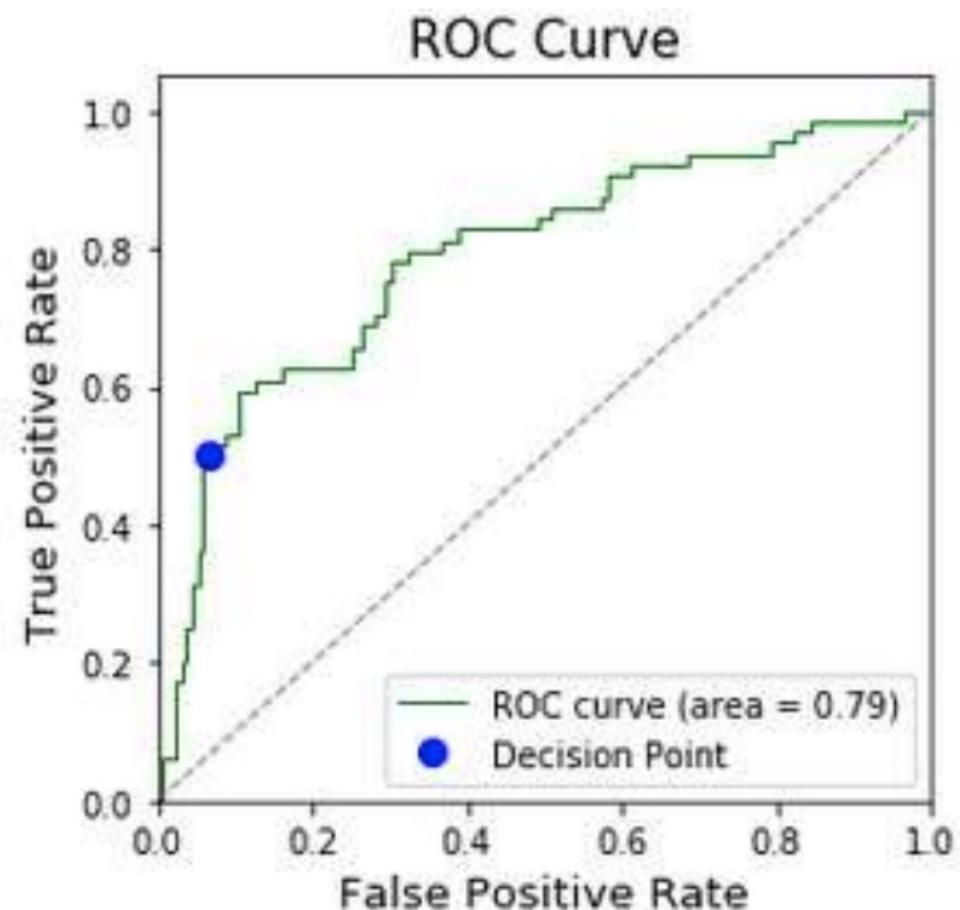


# Setting the Decision Threshold

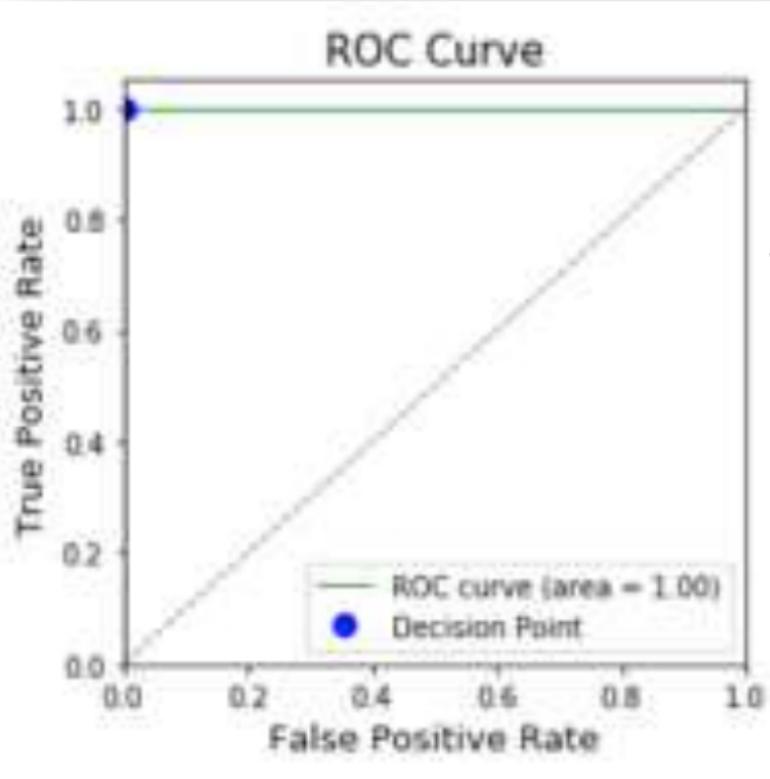


# Let's experiment with different decision thresholds

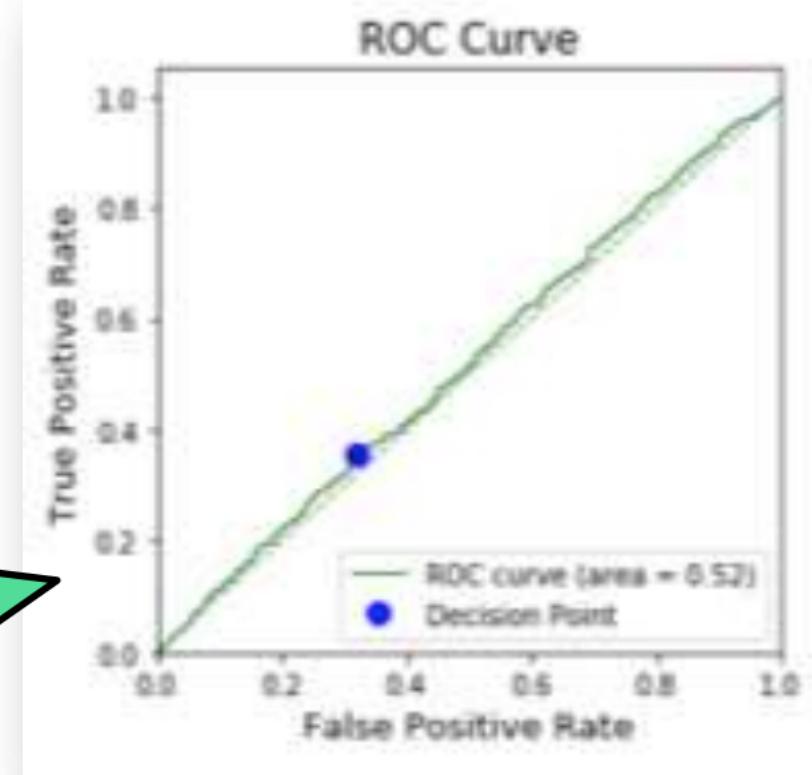
- The ‘Receiver Operating Characteristic’ (ROC) curve does just that ...
  - Systematically sweep through levels of decision threshold
  - Plot the ‘True Positive Rate’ vs. ‘False positive Rate’
- You decide your decision point based on what matters most



# What you should look for in your ROC?



**Perfect classifier**  
100% true positives,  
0% false positives



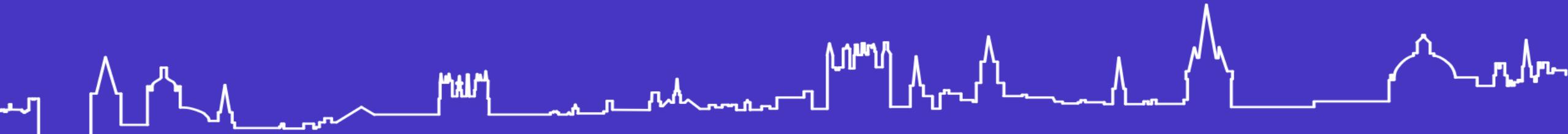
**Purely Random Classifier**  
Just as many false positives  
as true positives

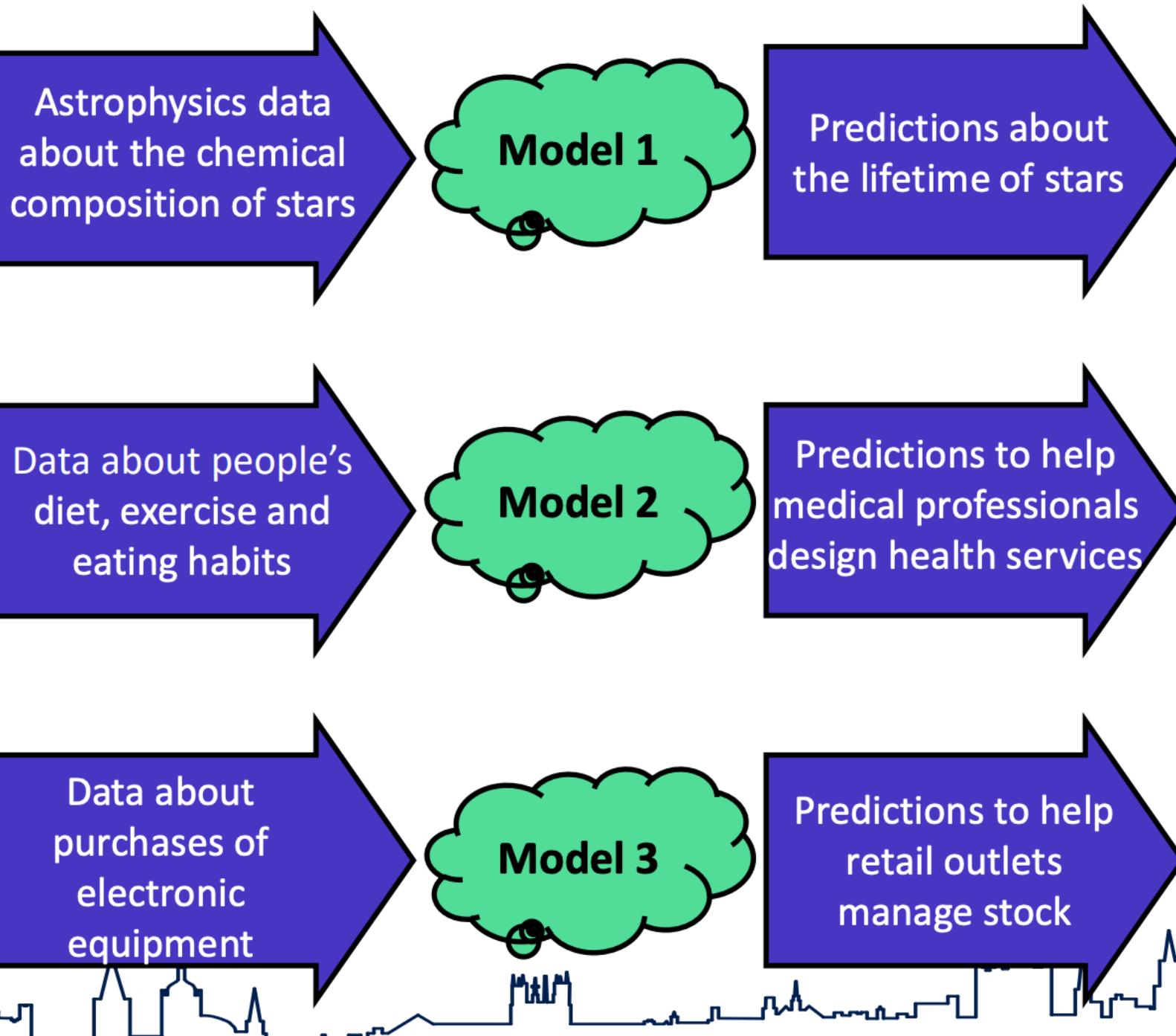


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# A Final Thought on Model Quality ..

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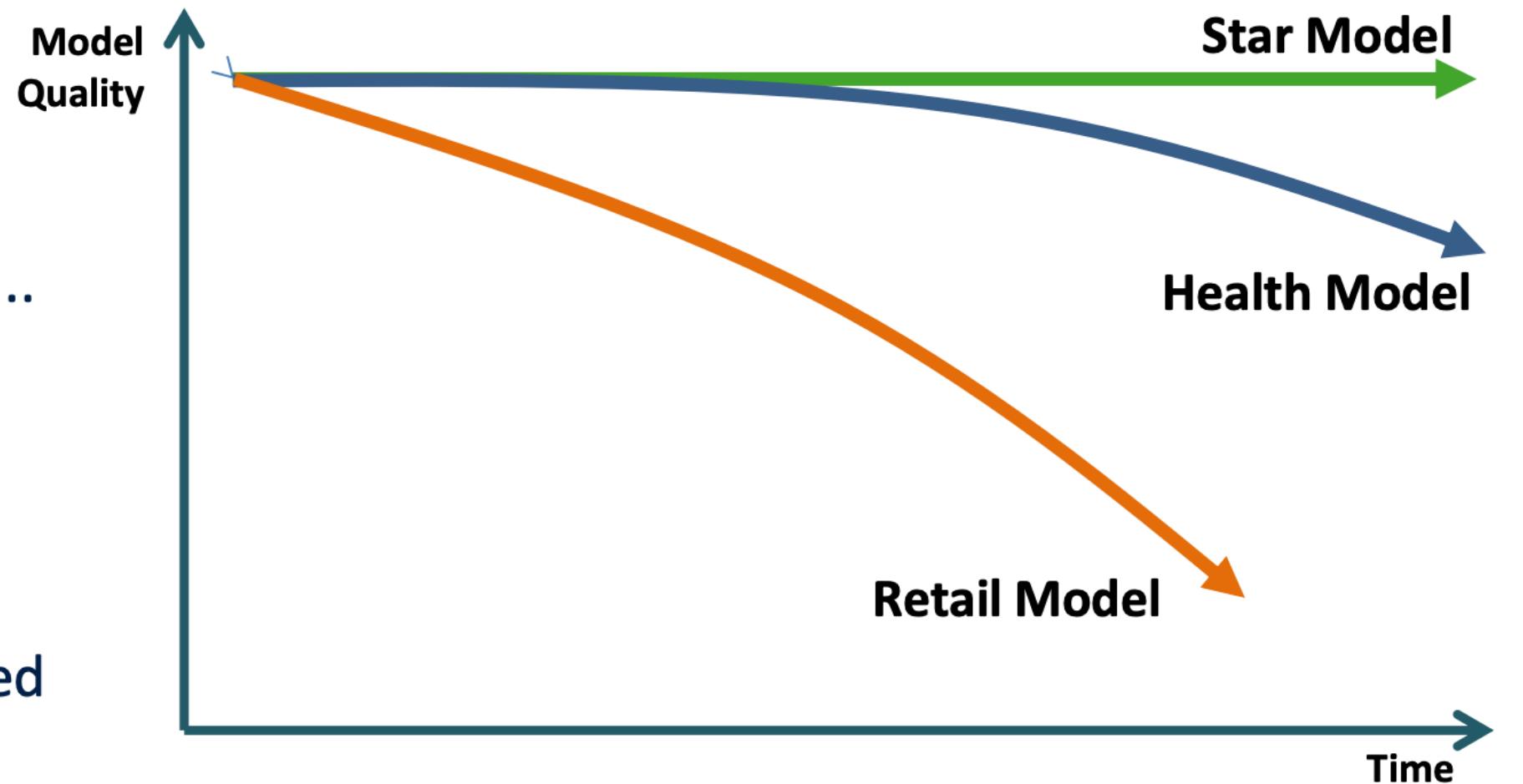


Thinking about measures of model quality ..

Why might we have to think differently about measuring quality of the three models on the left?

# How does model quality change over time?

- The real world changes over time ..
- Some things that were true yesterday .. May be less true today
- Real world data may change ..
- And models may need to be updated



# Models may need to be monitored and re-trained

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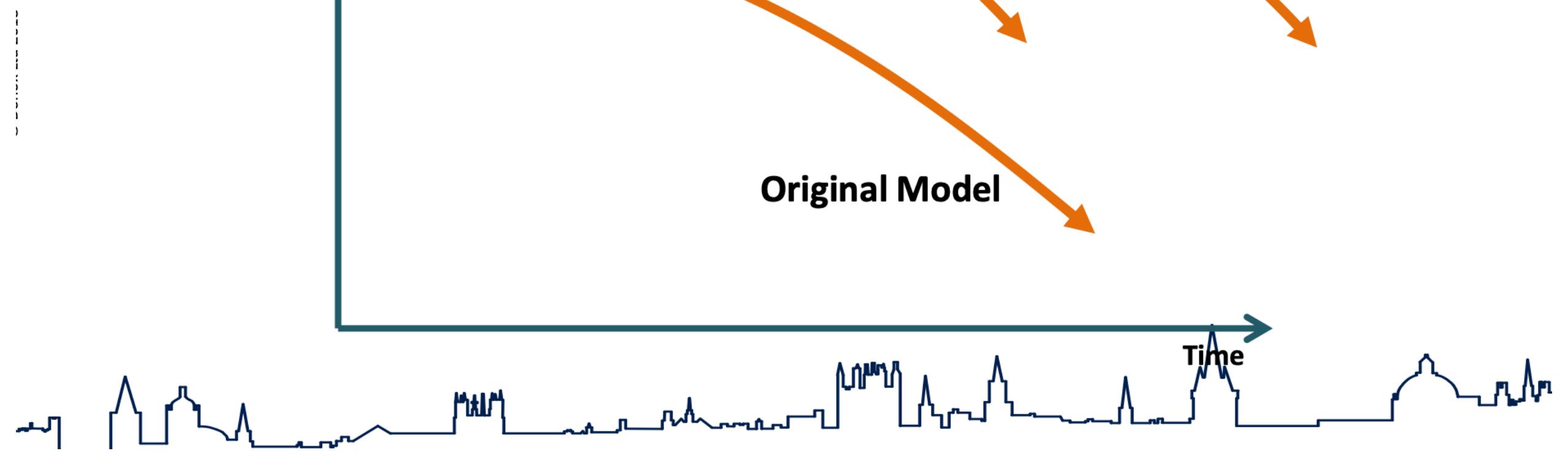
Model Quality

Re-trained model 1

Re-trained model 2

Original Model

Time



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# Conclusion

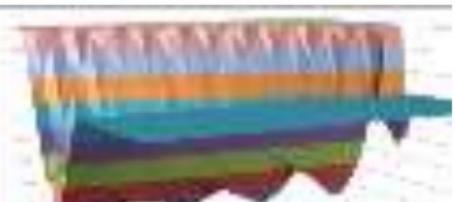
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# Machine Learning Fundamentals

# Concerned about curves

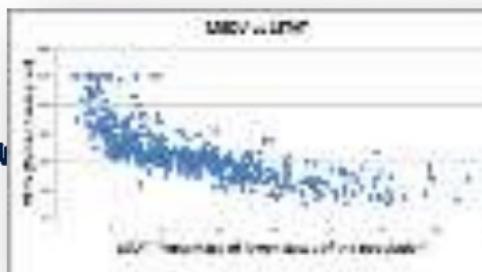
## Beyond straight-lines



# Reducing others



## Some curves are useful



## Tuning your Machine



# Shape matters



Making it  
easier to get fit



## How to get fit

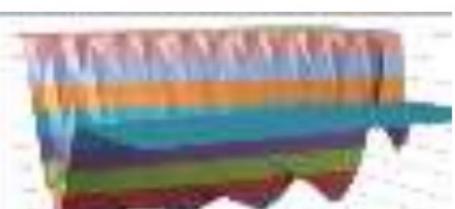
## How do algorithms actually fit models to data?

## Let's ROC

# Time to choose

## More about classification

# Some hills are too tough



# How to get Fat

## Working in higher-dimensions

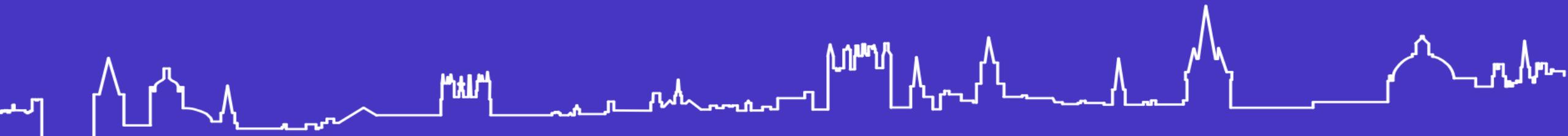


## Welcome to the Matrix

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# Out-takes (gag reel)

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# Lessons Learnt ..

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Always read the manual!

Trust your own knowledge, skill and insight

Don't assume that the model must be right

There may be more than one 'right' answer



		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) <b>Type II Error</b>	<b>Sensitivity</b> $\frac{TP}{(TP + FN)}$
	Negative	False Positive (FP) <b>Type I Error</b>	True Negative (TN)	<b>Specificity</b> $\frac{TN}{(TN + FP)}$
	Precision $\frac{TP}{(TP + FP)}$	Negative Predictive Value $\frac{TN}{(TN + FN)}$	Accuracy $\frac{TP + TN}{(TP + TN + FP + FN)}$	