Three faces of binary classification

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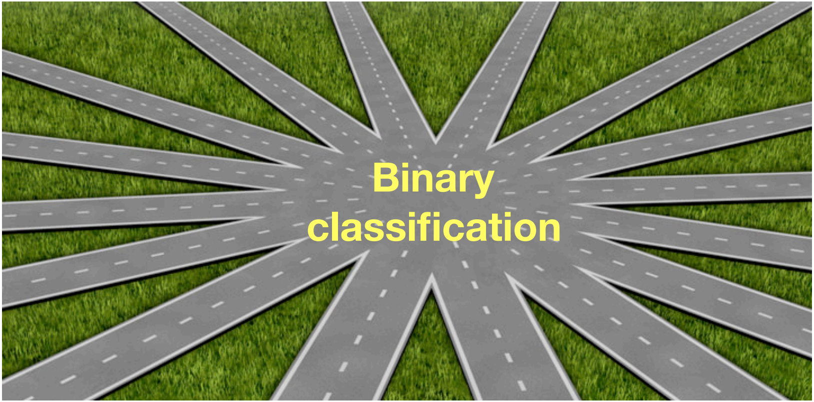
Today's lesson

All roads lead to binary classification



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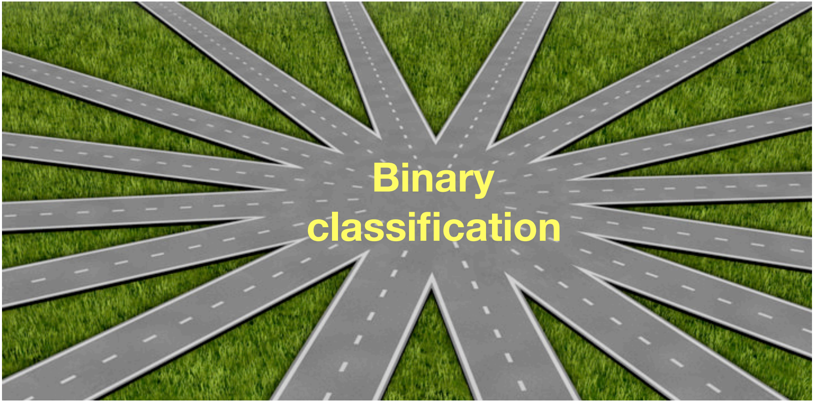

But what **is** binary classification, exactly?

Recap: binary classification

Goal: predict binary label $y \in \{0, 1\}$ for instance $\mathbf{x} \in \mathcal{X}$

- we call $y = 1$ the "positive" class, and $y = 0$ the "negative" class

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Recap: logistic regression

Logistic regression models the probability of an instance $\mathbf{x}$ belonging to the positive class $y = 1$

We posit this probability is

$$\mathbb{P}(y = 1 \mid \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}}}$$

Classify $\mathbf{x}$ as positive if $\mathbb{P}(y = 1 \mid \mathbf{x}) > 0.5$

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\pitchfork & & \pitchfork & & \pitchfork \\
\mathbb{R} & & [0,1] & & \{0,1\} \\
\text{Scores} & & \text{Probabilities} & & \text{Classifications}
\end{array}
$$

Classifiers, probability estimators, scorers

We may call a model:

$c\colon \mathcal{X} \to \{0,1\}$ a classifier

$p\colon \mathcal{X} \to [0,1]$ a probability estimator

$s\colon \mathcal{X} \to \mathbb{R}$ a scorer

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Logistic regression has a scorer

$$\begin{array}{c} s(\mathbf{x}) \\ \cap \\ \mathbb{R} \end{array}$$

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\cap & & \cap \\
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$$

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Logistic regression has a scorer, which is implicitly converted to a probability estimator, and then a classifier

$$\underset{\mathbb{R}}{\underset{\cap}{s(\mathbf{x})}} \longrightarrow \underset{[0,1]}{\underset{\cap}{\frac{1}{1+e^{-s(\mathbf{x})}}}} \longrightarrow \underset{\{0,1\}}{\underset{\cap}{\mathbf{1}\left[\frac{1}{1+e^{-s(\mathbf{x})}} > 0.5\right]}}$$

Where are they useful?

These models provide different things:

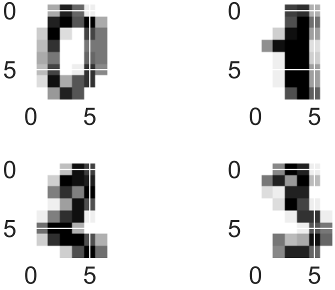
Classifiers	hard decisions
Probability-estimators	soft decisions (i.e., confidences)
Scorers	soft-er decisions (i.e., rankings)

Model types: example

Consider predicting if a digit is even or odd

```
(X, Y) = load_digits(return_X_y = True)

for i in range(0, 4):
    plt.subplot(2,2,i+1);
    plt.imshow(X[i,:].reshape((8,8)), cmap = plt.cm.
        gray_r, interpolation='nearest')
```



Model types: example

Consider predicting if a digit is even or odd

```
lrn = LogisticRegression()
lrn.fit(X, (Y % 2 == 0).astype(int))

print(lrn.predict(X[0,:].reshape(1,-1)))
print(lrn.predict_proba(X[0,:].reshape(1,-1))[:,1])
print(lrn.decision_function(X[0,:].reshape(1,-1)))
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```

gives:

`[1]` (classification)

`[0.99702005]` (probability)

`[5.81286542]` (score)

Are they really different?

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Care is needed when evaluating the different types of models

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Our model should discriminate between the two classes

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Our model should discriminate between the two classes

The precise meaning of “discriminate” varies:

Classifiers	have prediction equal to the target label
Probability-estimators	have probability close to the target label
Scorers	score positive instances higher than negative instances

Evaluating models: summary

The general principle for evaluation is:

Our model should discriminate between the two classes

The precise meaning of “discriminate” varies:

Classifiers	misclassification error
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Evaluating a classifier

Suppose one trains a classifier $c\colon \mathcal{X} \to \{0, 1\}$

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Natural thought: look at the misclassification error

$$\mathrm{ERR}(c) = \frac{1}{N} \sum_{n=1}^{N} \mathbf{1}[y_n \neq c(\mathbf{x}_n)],$$

i.e., the fraction of erroneous classifications

Evaluating a classifier: example

```
(X, Y) = load_digits(return_X_y = True)

...

XTr, XTe, YTr, YTe = train_test_split(X, (Y % 2 == 0).
    astype(int), random_state = 42)

lrn = LogisticRegression()
lrn.fit(XTr, YTr)

1 - accuracy_score(YTe, lrn.predict(XTe))
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We get a misclassification error of `6.7%`: pretty good!

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Suppose one trains a scorer $s \colon \mathcal{X} \to \mathbb{R}$

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We could look at either:

- how accurate our derived classifier is
- if our scores discriminate the two classes

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We'll return to the first option later

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We might measure this using the pairwise-disagreement:

$$\mathrm{PD}(s) = \frac{1}{N_0 \cdot N_1} \sum_{n \colon y_n = 1} \sum_{m \colon y_m = 0} \mathbf{1}[s(\mathbf{x}_n) < s(\mathbf{x}_m)]$$

where $N_i = \#$ instances with $y_n = i$

- fraction of positives scored below negatives

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We get a pairwise disagreement of `2.6%`: very good!

Evaluating a scorer

We get a different answer if we use pairwise disagreement to evaluate the classifier:

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We get a pairwise disagreement of $6.7\% \neq 2.6\%$!

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The general principle for evaluation is:

> Our model should discriminate between the two classes

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Roadmap

We'll look at how classification can be useful in:

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Application: imbalanced learning

Putting our skills to the test

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Natural thought: train a classifier!

Putting our skills to the test

```
M = loadmat('kddcup98.mat');
X = M['X']
Y = M['Y'].flatten()
XTr, XTe, YTr, YTe = train_test_split(X, Y, random_state
    = 42, test_size = 0.20)

lrn = LogisticRegression()
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```

We get a misclassification error of `5.0%`: very good!

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We confidently present our classifier to the company

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Unfortunately, a week later, they irately fire us

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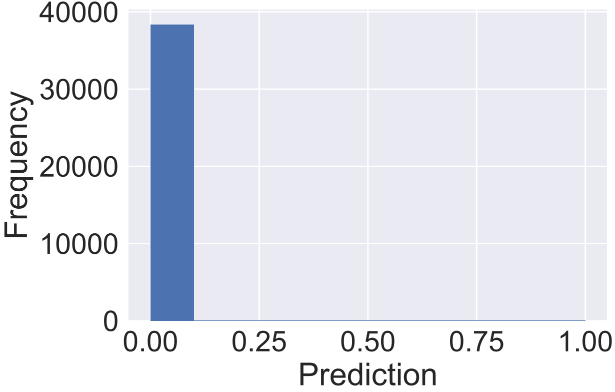

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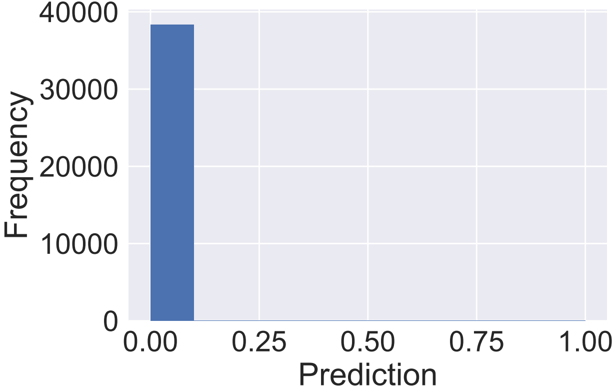

We ended up predicting that no one should be sent a flier!

Evaluating a classifier: revisited

Recall that we proposed to compute:

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$$\mathrm{ERR}(c) = \frac{N_1}{N},$$

where N_1 is the # of instances with $y_n = 1$

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Since $N_1 \ll N$, the error rate will be very low!

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To unwrap this, we could compute the per-class error rates,

$$\mathrm{ERR}_1(c) = \frac{1}{N_1} \sum_{n:\, y_n = 1} \mathbf{1}[y_n \neq c(\mathbf{x}_n)]$$

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These are known as the false negative and false positive rates

Weighted misclassification error

Standard misclassification error is:

$$\mathrm{ERR}(c) = p \cdot \mathrm{ERR}_1(c) + (1-p) \cdot \mathrm{ERR}_0(c),$$

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Consider instead a cost-weighted error

$$\mathrm{ERR}(c) = w \cdot \mathrm{ERR}_1(c) + (1-w) \cdot \mathrm{ERR}_0(c),$$

for $w \in [0,1]$ the relative importance of per-class errors

Putting our skills to the test: revisited

```
C = confusion_matrix(YTe, lrn.predict(XTe))
w = 0.5
w * C[0,1] + (1 - w) * C[1,1]
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We get a weighted error rate of `50%`: that sounds very bad!

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More abstractly, we are summarising a confusion matrix

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We could also try to evaluate our underlying scorer:

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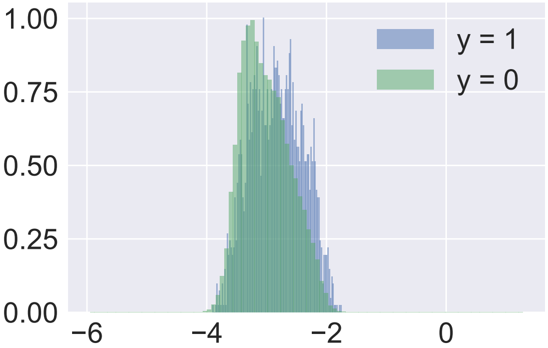
We get a pairwise disagreement of `38.2%`: not great, but not trivial either!

Distribution of scores

There is a slight gap between $y = 1$ and $y = 0$ amongst the scores



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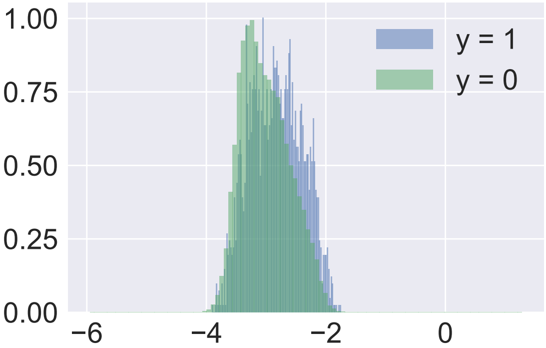

But also note that all the scores are < 0!

- we are picking a bad threshold to form a classifier!

ROC curves

Given a scorer s, we could make a classifier c_t using any $t \in \mathbb{R}$:

$$c_t(\mathbf{x}) = \mathbf{1}[s(\mathbf{x}) > t]$$

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The ROC curve is a plot of the resulting false versus true positives, as t is varied:

$$\{(\mathrm{ERR}_0(c_t), 1 - \mathrm{ERR}_1(c_t)) : t \in \mathbb{R}\}$$

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Given a scorer s, we could make a classifier c_t using any $t \in \mathbb{R}$:

$$c_t(\mathbf{x}) = \mathbf{1}[s(\mathbf{x}) > t]$$

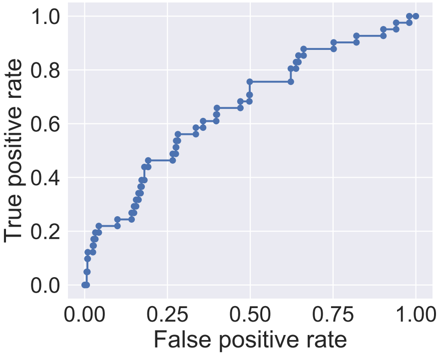
The ROC curve is a plot of the resulting false versus true positives, as t is varied:

$$\{(\mathrm{ERR}_0(c_t), 1 - \mathrm{ERR}_1(c_t)) \colon t \in \mathbb{R}\}$$

This is a graphical summary of all possible classifiers we could obtain by thresholding s

ROC curves: example

```
fpr, tpr, thresholds = roc_curve(YTe, lrn.
    decision_function(XTe), pos_label = 1)
plt.plot(fpr, tpr, '.-', markersize = 12);
```



Any point on this curve corresponds to a single classifier c_t

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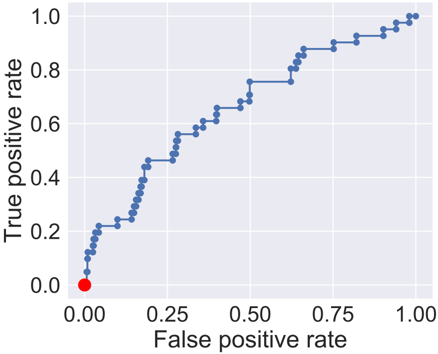

Trivial “always negative” classifier: weighted error `50%`

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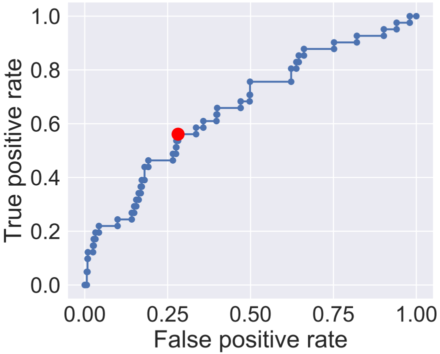

Better classifier: weighted error `36%`

ROC and pairwise disagreement

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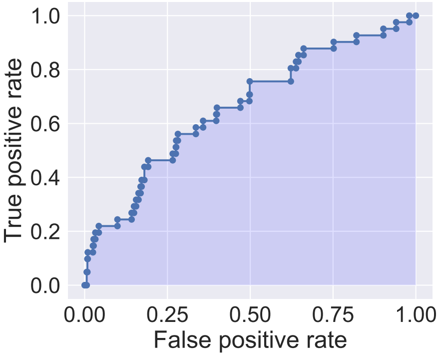
It turns out that pairwise disagreement is one minus the area under the ROC curve

Intuitively, average performance of collection $\{c_t : t \in \mathbb{R}\}$



Roadmap

We'll look at how classification can be useful in:

- predicting rare events
- imputing missing data (by creating features)
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Application: matrix factorisation

Item response modelling

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The examiners prepared a number of different questions

Each student was give a different subset of these questions

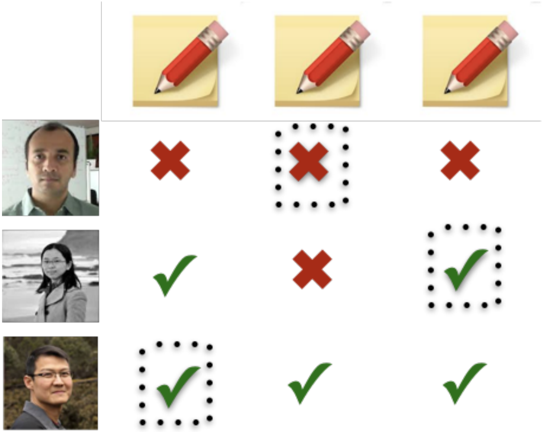
They want to standardise performance across students

Item response modelling: goal

How to account for the fact that some students may have gotten an easy batch of questions?

Item response modelling: strategy

We want to predict how well a student would do on all other questions they weren't asked



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We want a classifier $c \colon \mathcal{X} \to \{0, 1\}$

- use this to predict unseen (student, question) outcomes

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How can we construct a classifier without any features?!

We can try to learn good features from the data!

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Here, $\mathbf{u}_s$ and $\mathbf{v}_q$ are learned features for the student and question respectively

Training the probability-estimator

For fixed question features $\mathbf{v}_q$,

$$\mathbb{P}(y = 1 \mid \mathbf{x}) = \frac{1}{1 + e^{-{\mathbf{u}_s}^{\mathrm{T}} \mathbf{v}_q}}$$

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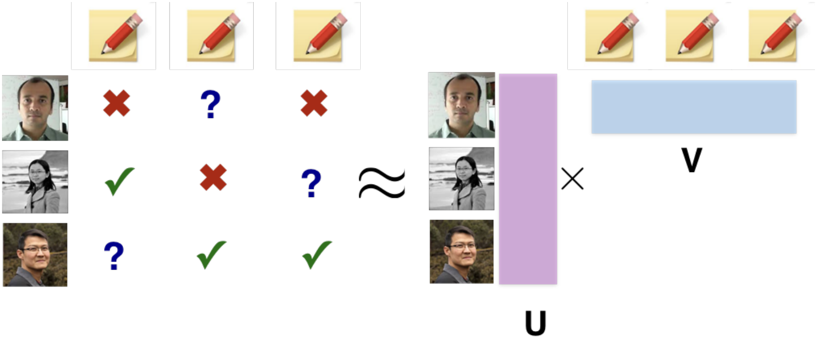
We can fit the model by alternating optimisation:

- fix $\{\mathbf{u}_s\}$, and then fit $\{\mathbf{v}_q\}$ via logistic regression
- fix $\{\mathbf{v}_q\}$, and then fit $\{\mathbf{u}_s\}$ via logistic regression
- iterate till convergence

Matrix factorisation view

This can also be understood as a form of nonlinear matrix factorisation (c.f. PCA)



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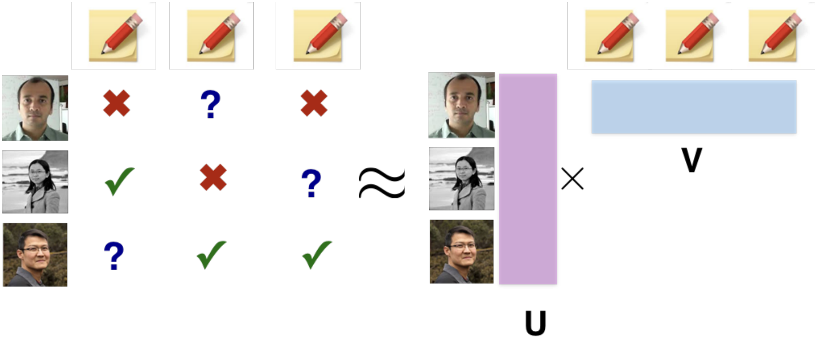

Compared to e.g. PCA, account for missing data

Other applications

Same idea applicable for recommender systems

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Application: GANs

Generative models

Suppose we want a model that can generate images

From https://medium.com/@ageitgey/abusing-generative-adversarial-networks-to-make-8-bit-pixel-art-e45d9b96cee7

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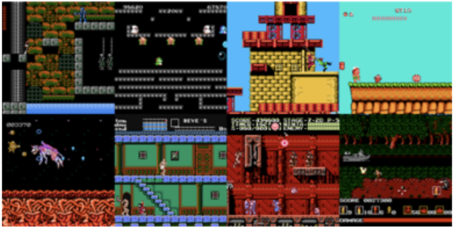
e.g., from Nintendo game backgrounds



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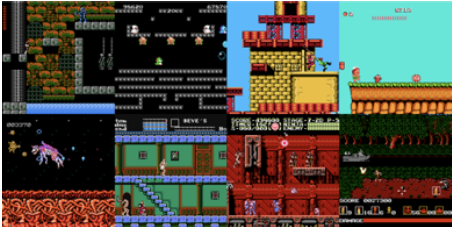
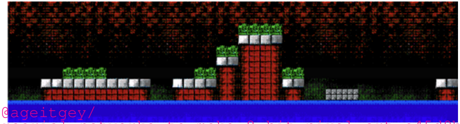


to the background for a new game



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Generative models: formally

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We want a generator $g : \mathcal{Z} \to \mathcal{X}$

We then draw samples $\{g(\mathbf{z}_m)\}_{m=1}^M$, for random seed vectors $\mathbf{z}_m$

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There are no labels available as input

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Hence, we can't possibly treat this as a classification problem

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Hence, we can’t possibly treat this as a classification problem

Unless we create some labels ourselves!

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Suppose we have generator $g \colon \mathcal{Z} \to \mathcal{X}$, and we draw $\{g(\mathbf{z}_m)\}_{m=1}^M$

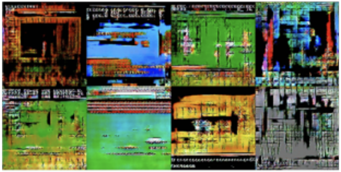
How do we tell if g is good, or not?

Find a classifier to distinguish between $\{\mathbf{x}_n\}_{n=1}^N$ and $\{g(\mathbf{z}_m)\}_{m=1}^M$!

- if a powerful classifier can't tell the difference, then probably humans can't either!

A classification perspective

Generated images



versus

True images

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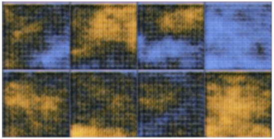
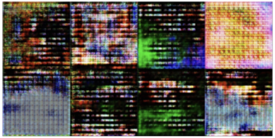
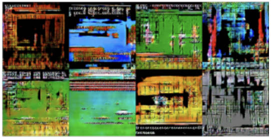
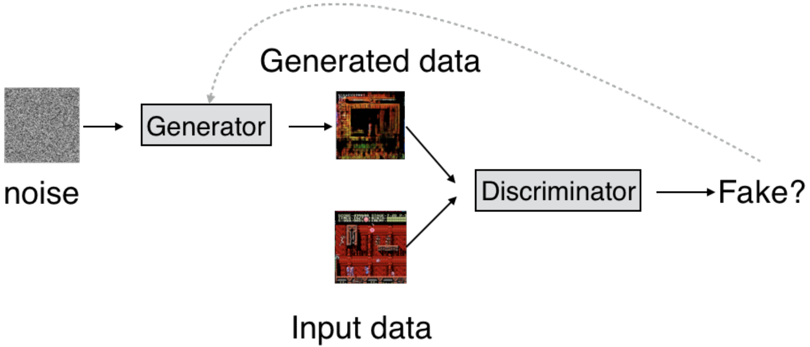






GANs summary

Can think of our procedure as a game between the generator and a discriminator (classifier)



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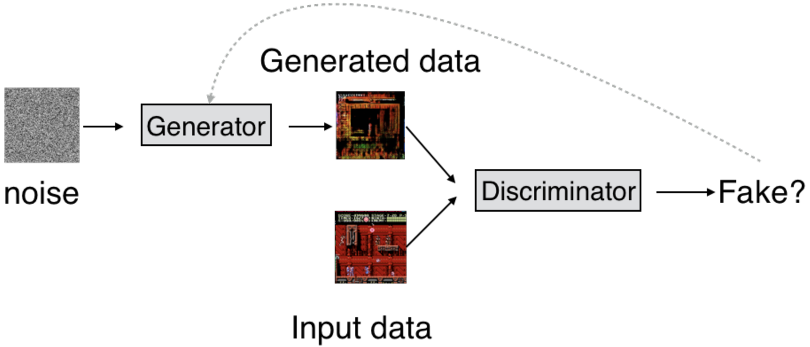

Generative adversarial networks (GANs) implement this idea with neural networks for the generator and discriminator

GAN examples

CAN: Creative Adversarial Networks Generating “Art” by Learning About Styles and Deviating from Style Norms. Elgammal et al., ICCC 2017.

GAN examples

Image-to-Image Translation with Conditional Adversarial Networks. Isola et al., CVPR 2017.

Final thoughts

Summary

Three views of classification

Evaluating classifiers

How classification can be useful in:

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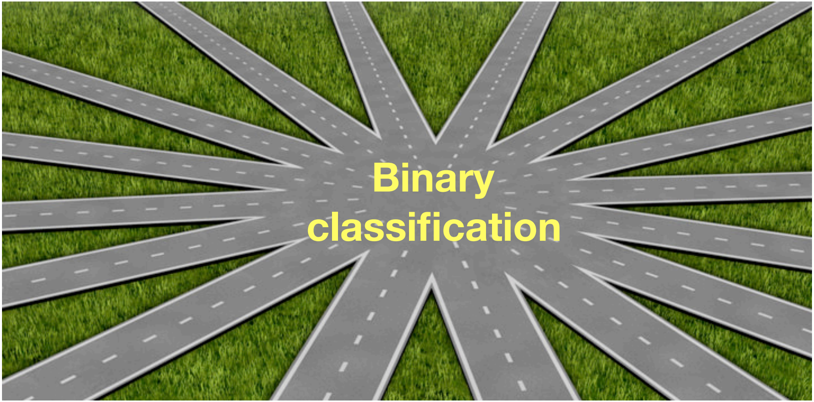
Today's lesson

All roads lead to binary classification



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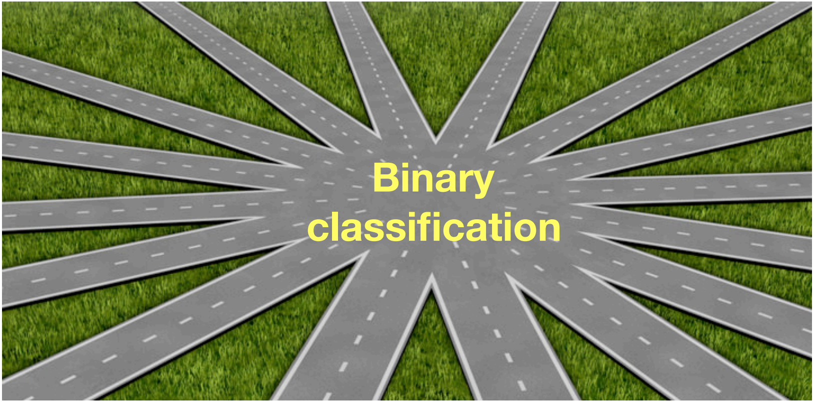

But we need to be careful in defining what "classification" is!