CPSC 340:
Machine Learning and Data Mining

Ensemble Methods

Fall 2018

Admin

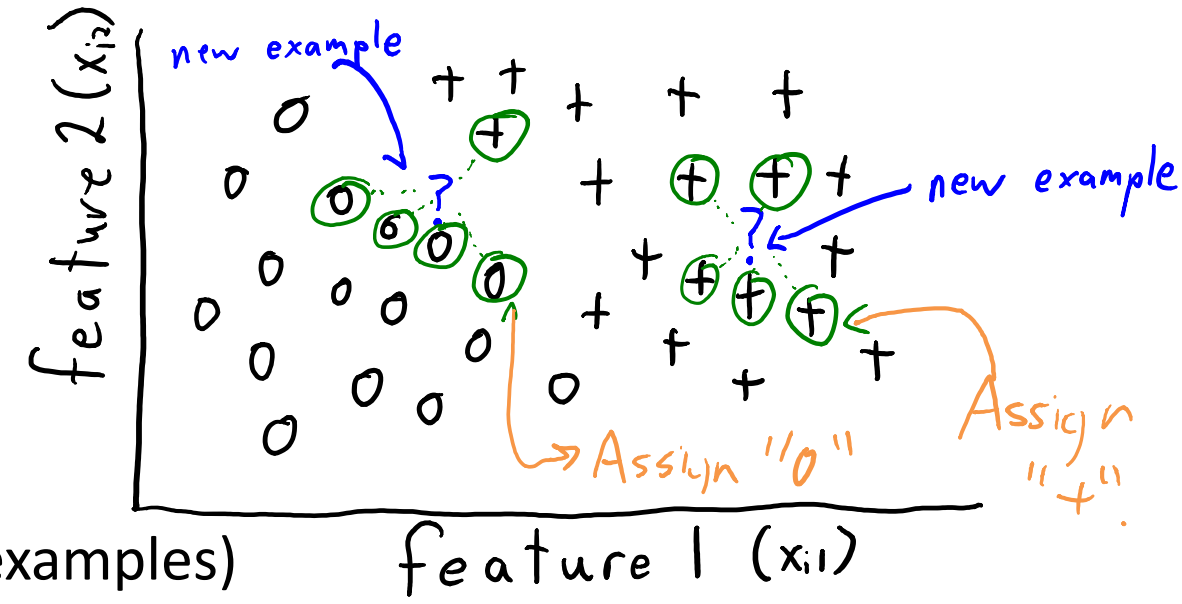
- Welcome to the course!
- Course webpage: www.ugrad.cs.ubc.ca/~cs340
- Assignment 2 is out.
  - Due Friday of next week. It's long so start early.

Last Time: K-Nearest Neighbours (KNN)

- K-nearest neighbours algorithm for classifying $\tilde{x}_i$:
  - Find 'k' values of x_i that are most similar to $\tilde{x}_i$.
  - Use mode of corresponding y_i.

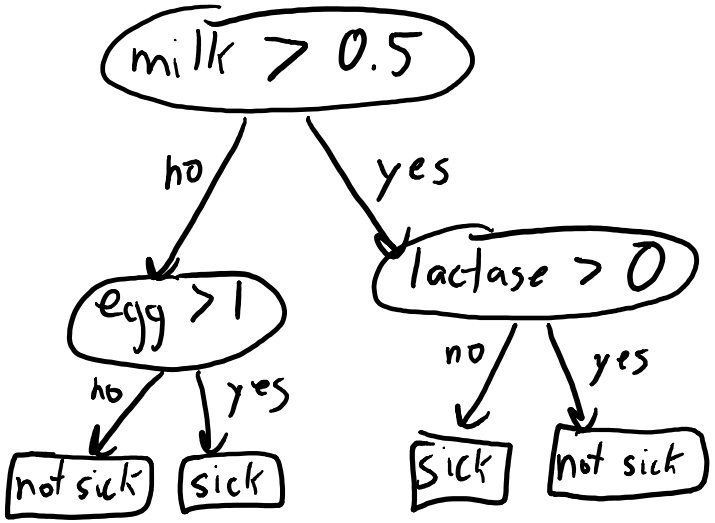
- Lazy learning:
  - To "train" you just store X and y.

- Non-parametric:
  - Size of model grows with 'n' (number of examples)
  - Nearly-optimal test error with infinite data.



- But high prediction cost and may need large 'n' if 'd' is large.

Decision Trees vs. Naïve Bayes vs. KNN

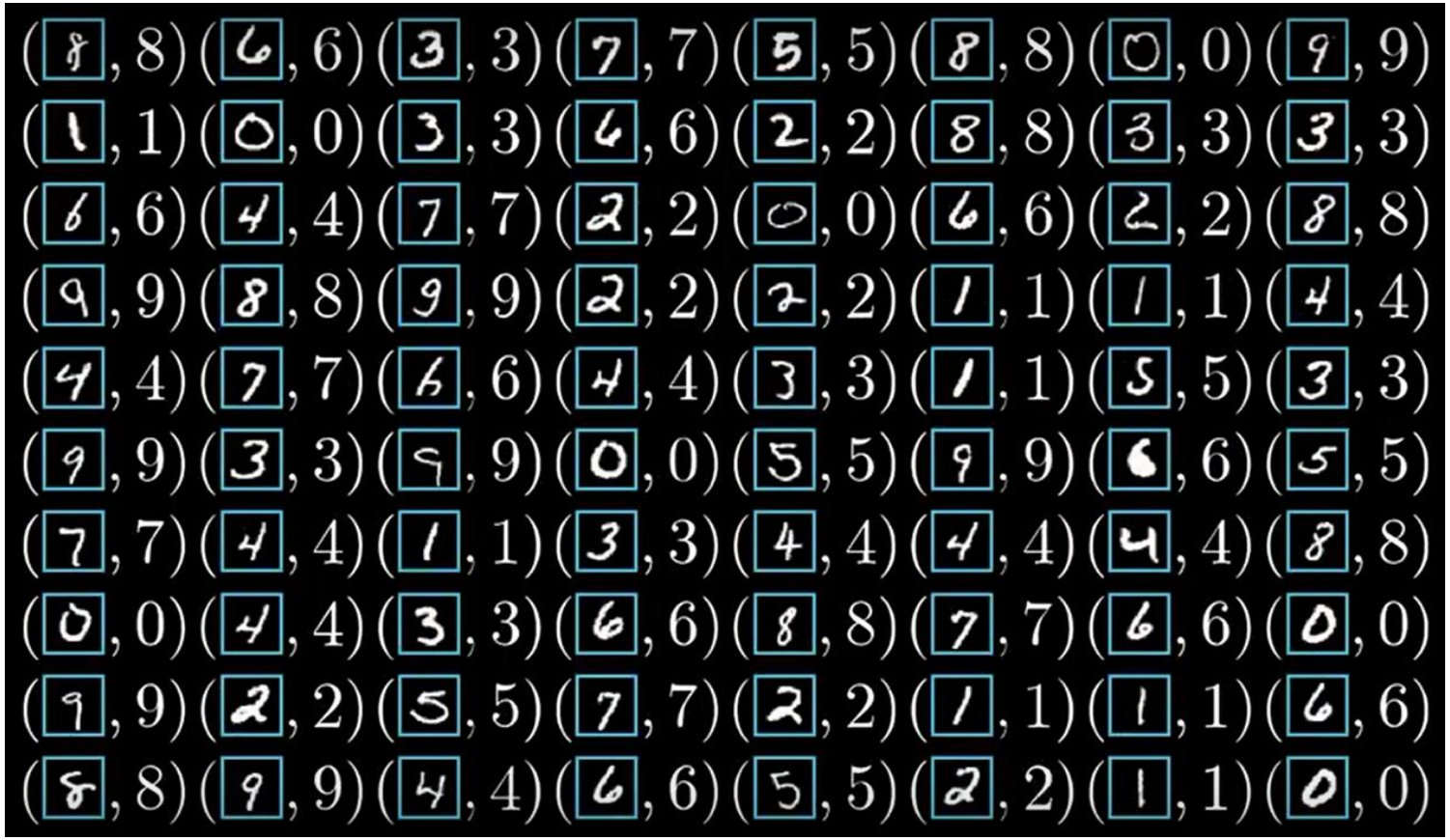


$$p(\text{sick} \mid \text{milk}, \text{egg}, \text{lactase}) \approx p(\text{milk} \mid \text{sick})\, p(\text{egg} \mid \text{sick})\, p(\text{lactase} \mid \text{sick})\, p(\text{sick})$$

(milk = 0.6, egg = 2, lactase = 0, ??) is close to
(milk = 0.7, egg = 2, lactase = 0, sick) so predict sick.

Application: Optical Character Recognition

- To scan documents, we want to turn images into characters:
  - "Optical character recognition" (OCR).



https://www.youtube.com/watch?v=IHZwWFHWa-w

Application: Optical Character Recognition

- To scan documents, we want to turn images into characters:
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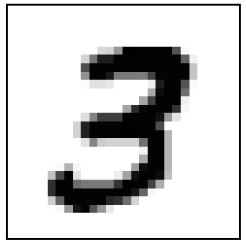


"3"

  - Turning this into a supervised learning problem (with 28 by 28 images):

$X =$

(1,1)	(2,1)	(3,1)	…	(28,1)	(1,2)	(2,2)	…	(14,14)	…	(28,28)
0	0	0		0	0	0		1		0
0	0	0		0	0	0		1		0
0	0	0		0	0	0		0		0
0	0	0		0	0	0		1		0

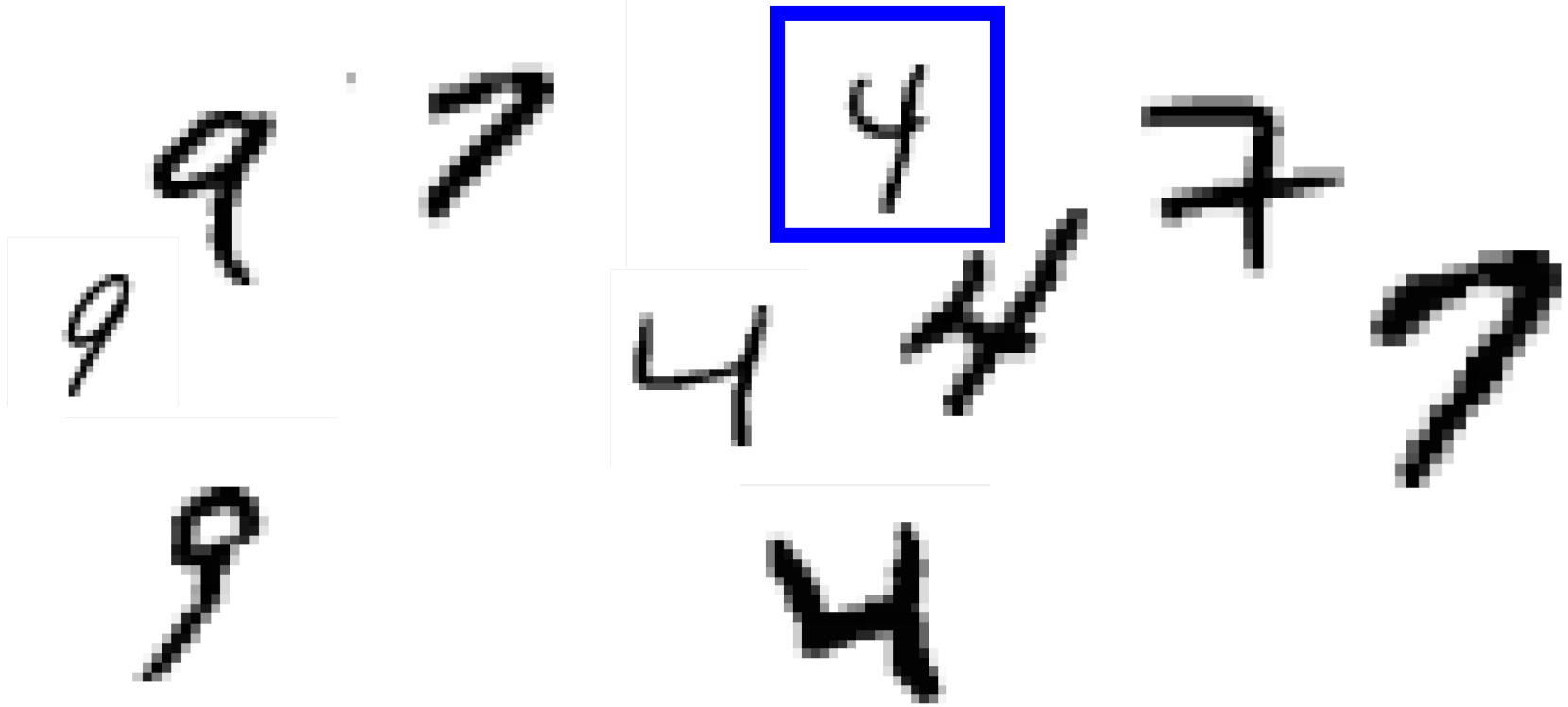
Each feature is grayscale intensity of one of the 784 pixels

$y =$

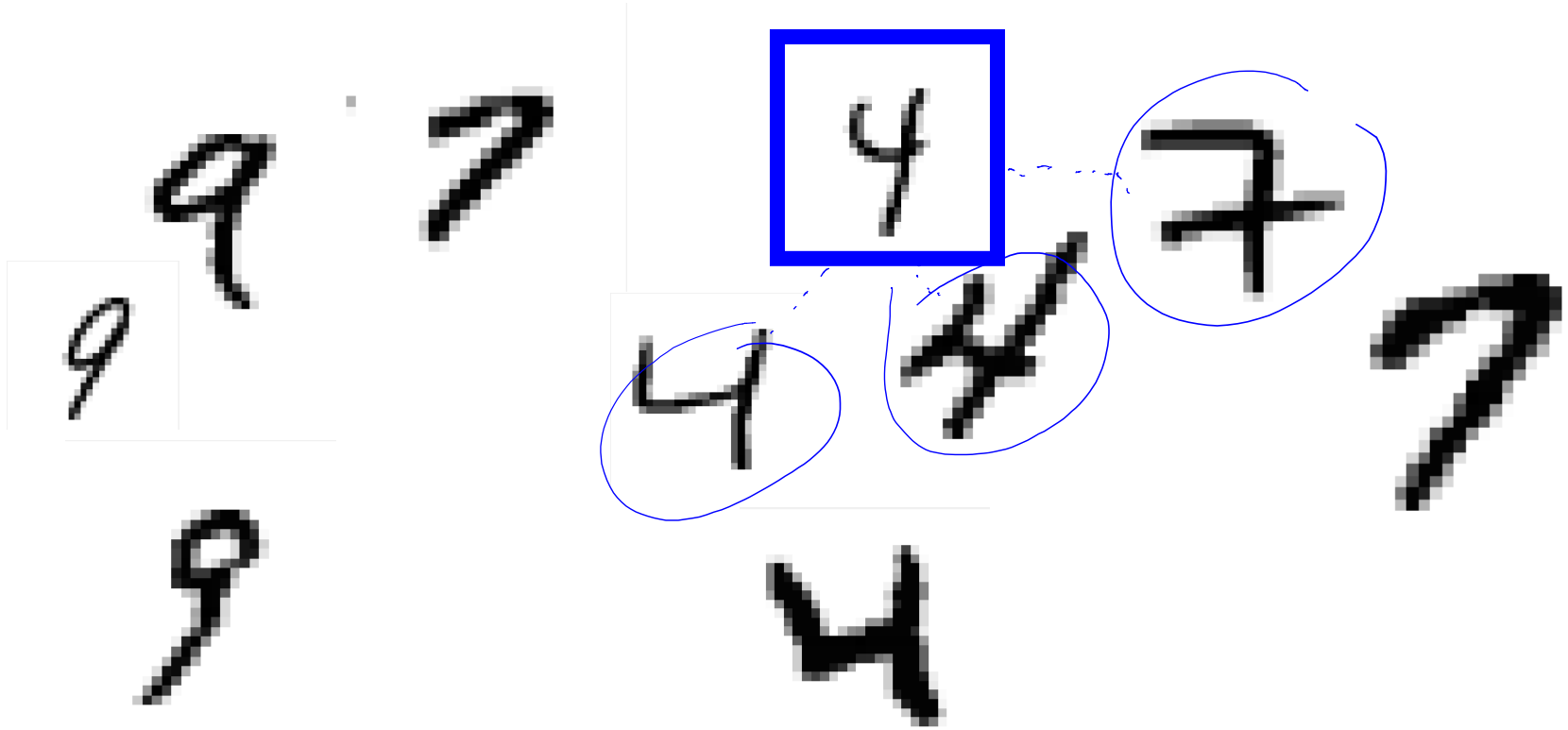
char
3
6
0
9

KNN for Optical Character Recognition

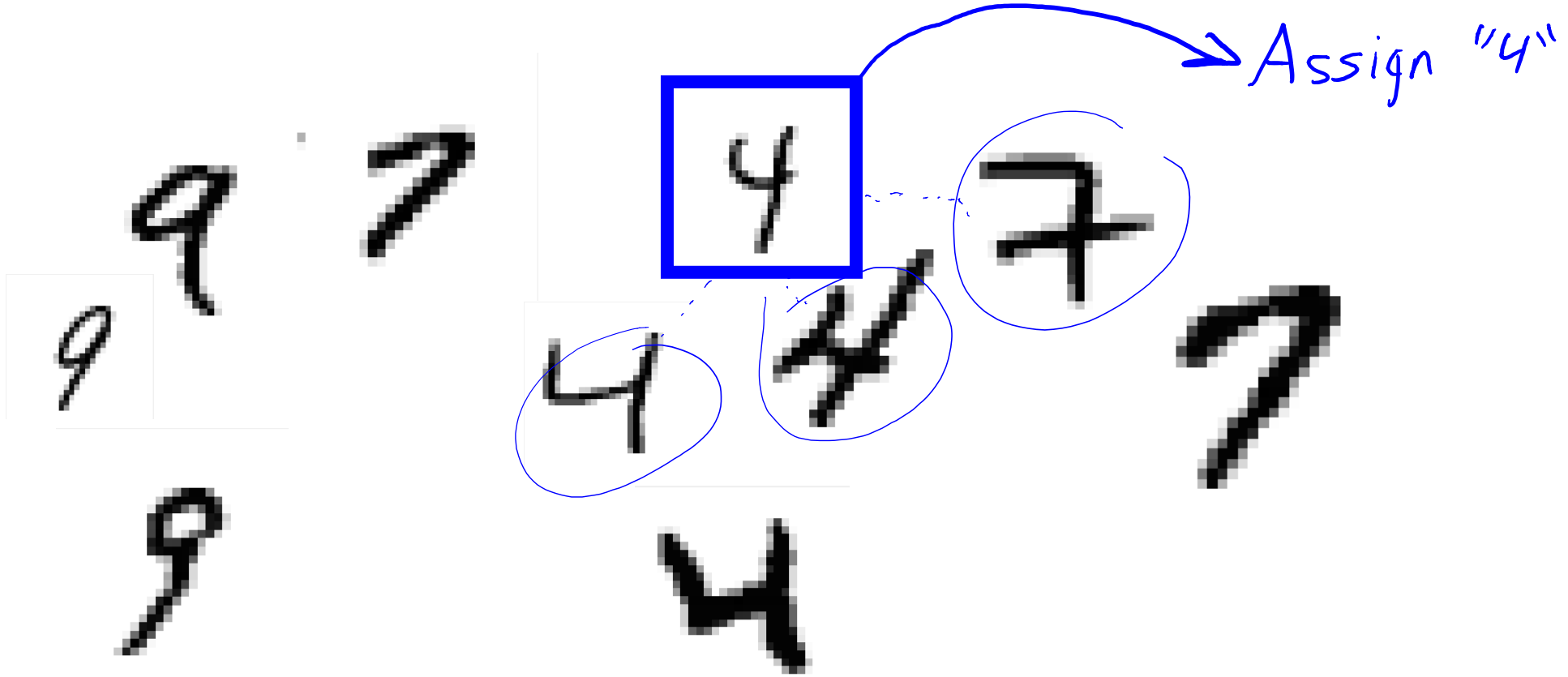
KNN for Optical Character Recognition



KNN for Optical Character Recognition



KNN for Optical Character Recognition



Human vs. Machine Perception

- There is huge difference between what we see and what KNN sees:

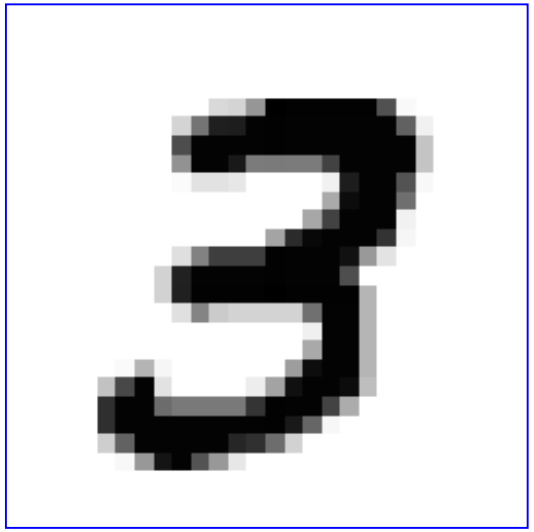
What we see:

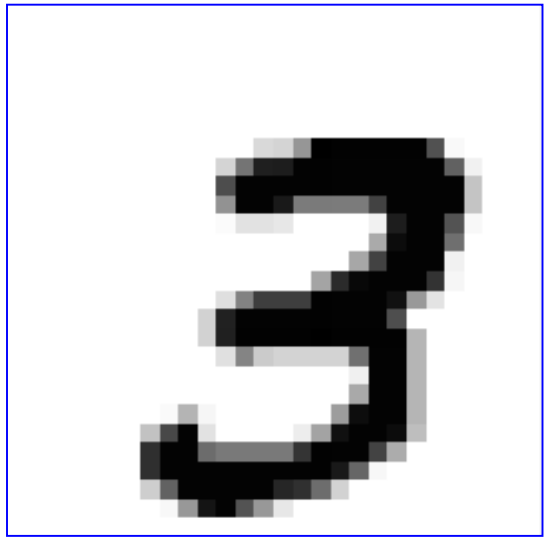
What the computer “sees”:

Actually, it’s worse:

What the Computer Sees

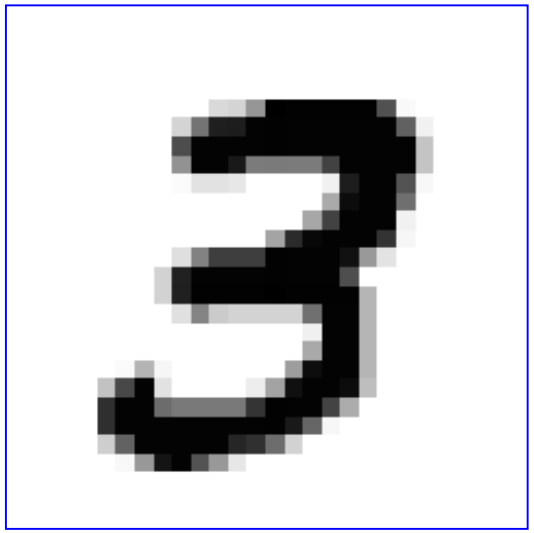
- Are these two images “similar”?

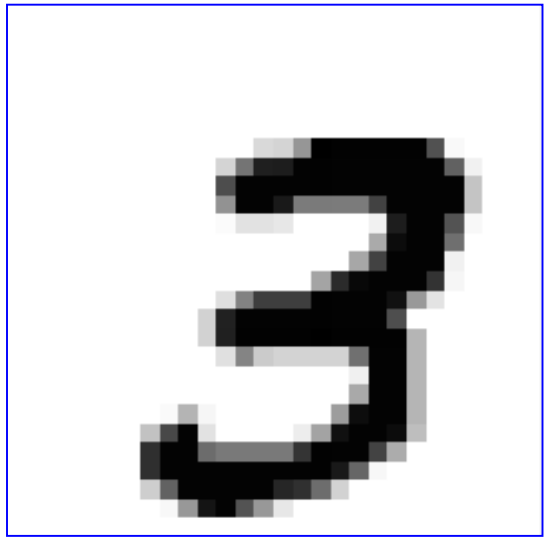




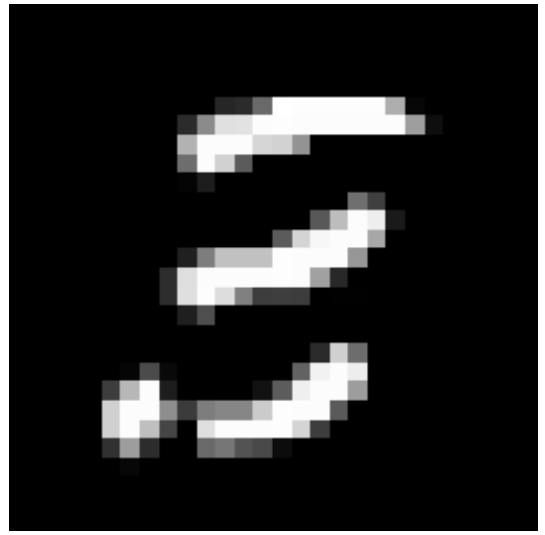
What the Computer Sees

- Are these two images “similar”?





Difference:

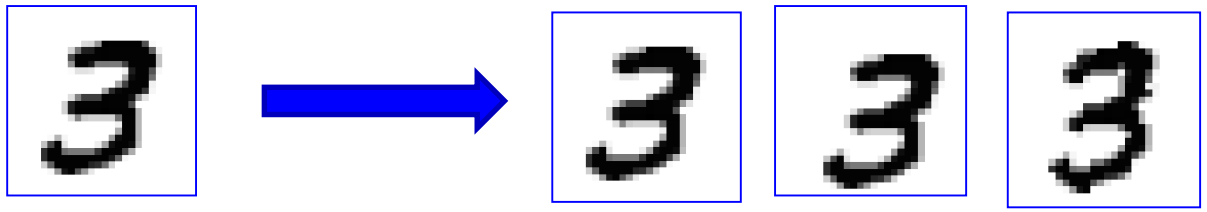


- KNN does not know that labels should be translation invariant.

Encouraging Invariance

- May want classifier to be invariant to certain feature transforms.
  - Images: translations, small rotations, changes in size, mild warping,…
- The hard/slow way is to modify your distance function:
  - Find neighbours that require the ‘smallest’ transformation of image.

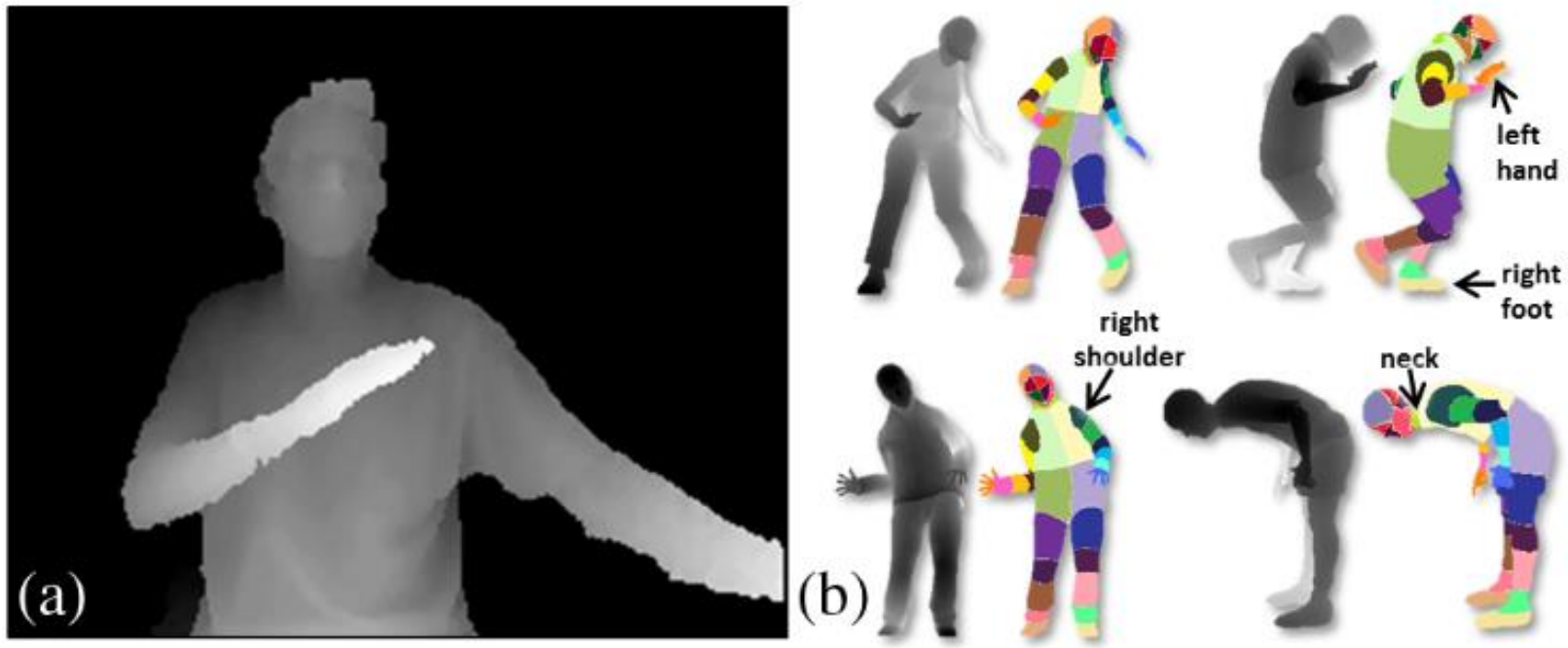
- The easy/fast way is to just add transformed data during training:
  - Add translated/rotate/resized/warped versions of training images.



  - Crucial part of many successful vision systems.
  - Also really important for sound (translate, change volume, and so on).

Application: Body-Part Recognition

- Microsoft Kinect:
  - Real-time recognition of 31 body parts from laser depth data.



- How could we write a program to do this?

http://research.microsoft.com/pubs/158806/CriminisiForests_FoundTrends_2011.pdf

Some Ingredients of Kinect

1. Collect hundreds of thousands of labeled images (motion capture).
   - Variety of pose, age, shape, clothing, and crop.
2. Build a simulator that fills space of images by making even more images.

3. Extract features of each location, that are cheap enough for real-time calculation (depth differences between pixel and pixels nearby.)
4. Treat classifying body part of a pixel as a supervised learning problem.
5. Run classifier in parallel on all pixels using graphical processing unit (GPU).

http://research.microsoft.com/pubs/145347/BodyPartRecognition.pdf

Supervised Learning Step

- ALL steps are important, but we'll focus on the learning step.

- Do we have any classifiers that are accurate and run in real time?
  - Decision trees and naïve Bayes are fast, but often not very accurate.
  - KNN is often accurate, but not very fast.

- Deployed system uses an ensemble method called random forests.

Ensemble Methods

- Ensemble methods are classifiers that have classifiers as input.
  - Also called “meta-learning”.
- They have the best names:
  - Averaging.
  - Boosting.
  - Bootstrapping.
  - Bagging.
  - Cascading.
  - Random Forests.
  - Stacking.
- Ensemble methods often have higher accuracy than input classifiers.

Ensemble Methods

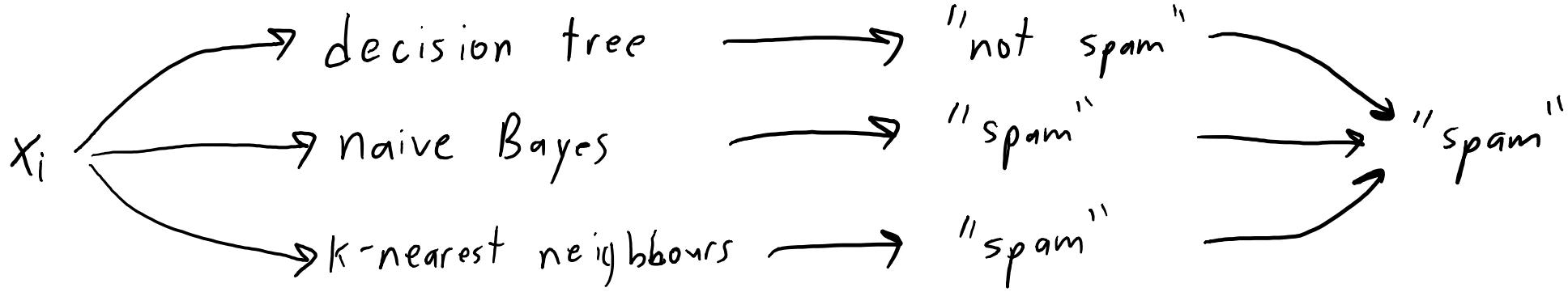
- Remember the fundamental trade-off:
  1. E_{train}: How small you can make the training error.

     vs.

  2. E_{approx}: How well training error approximates the test error.
- Goal of ensemble methods is that meta-classifier:
  - Does much better on one of these than individual classifiers.
  - Doesn't do too much worse on the other.
- This suggests two types of ensemble methods:
  1. Boosting: improves training error of classifiers with high E_{train}.
  2. Averaging: improves approximation error of classifiers with high E_{approx}.

Averaging

- Input to averaging is the predictions of a set of models:
  - Decision trees make one prediction.
  - Naïve Bayes makes another prediction.
  - KNN makes another prediction.
- Simple model averaging:
  - Take the mode of the predictions (or average probabilities if probabilistic).



Why can Averaging Work?

- Why can averaging lead to better results?

- Consider classifiers that overfit (like deep decision trees):
  - If they all overfit in exactly the same way, averaging does nothing.

- But if they make independent errors:
  - Probability of error of average can be lower than individual classifiers.
  - Less attention to specific overfitting of each classifier.

Why can Averaging Work?

- Consider 3 binary classifiers, each independently correct with probability 0.80:

- The ensemble will be correct if the of the 3 mode is right ("3 right" or "2 right").
  - P(all 3 right) = 0.8^3 = 0.512.
  - P(2 rights, 1 wrong) = $3*0.8^2(1-0.8)$ = 0.384.
  - P(1 right, 2 wrongs) = $3*(1-0.8)^2 0.8$ = 0.096.
  - P(all 3 wrong) = $(1-0.8)^3$ = 0.008.
  - So ensemble is right with probability 0.896 (which is 0.512+0.384).

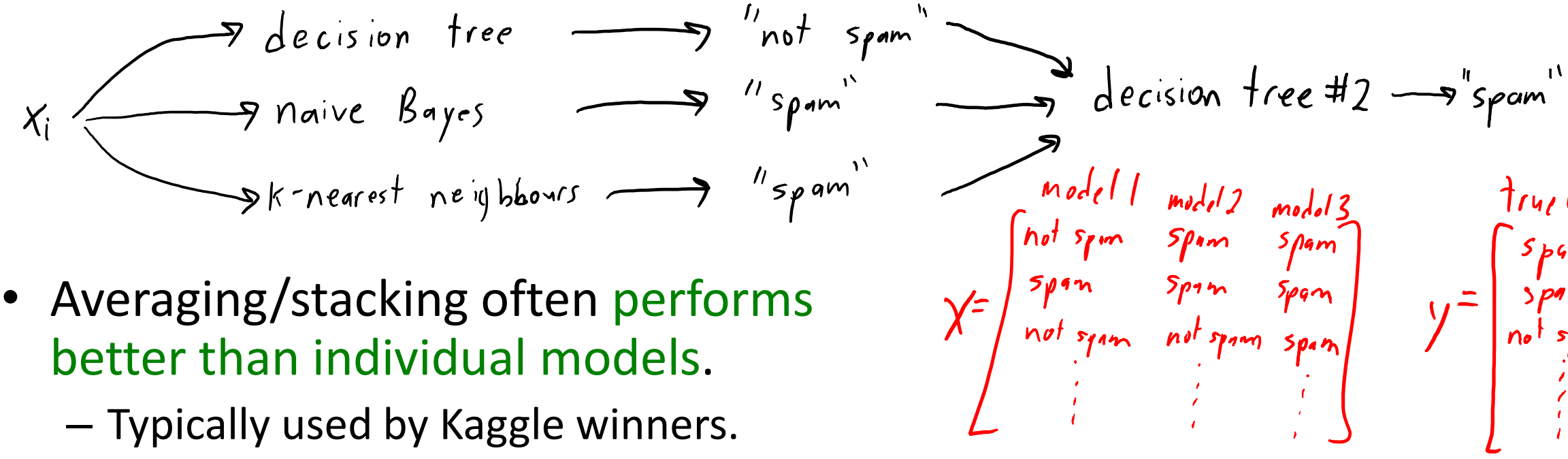
- Notes:
  - For averaging to work, classifiers need to be at least somewhat independent.
  - You also want the probability of being right to be > 0.5, otherwise it will do much worse.
  - Probabilities also shouldn't be to different (otherwise, it might be better to take most accurate).

Averaging

- Consider a set of classifiers that make these predictions:
  - Classifier 1: “spam”.
  - Classifier 2: “spam”.
  - Classifier 3: “spam”.
  - Classifier 4: “not spam”.
  - Classifier 5: “spam”.
  - Classifier 6: “not spam”.
  - Classifier 7: “spam”.
  - Classifier 8: “spam”.
  - Classifier 9: “spam”.
  - Classifier 10: “spam”.
- If these independently get 80% accuracy, mode will be close to 100%.
  - In practice errors won’t be completely independent (due to noise in labels).

Stacking

- Stacking:
  - Fit another classifier that uses the predictions as features.



- Averaging/stacking often performs better than individual models.
  - Typically used by Kaggle winners.
  - E.g., Netflix $1M user-rating competition winner was stacked classifier.

Random Forests

- Random forests average a set of deep decision trees.
  - Tend to be one of the best "out of the box" classifiers.
    - Often close to the best performance of any method on the first run.
  - And predictions are very fast.

- Do deep decision trees make independent errors?
  - No: with the same training data you'll get the same decision tree.

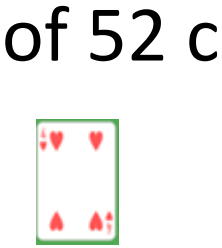
- Two key ingredients in random forests:
  - Bootstrapping.
  - Random trees.

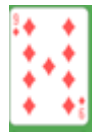
Boostrap Sampling

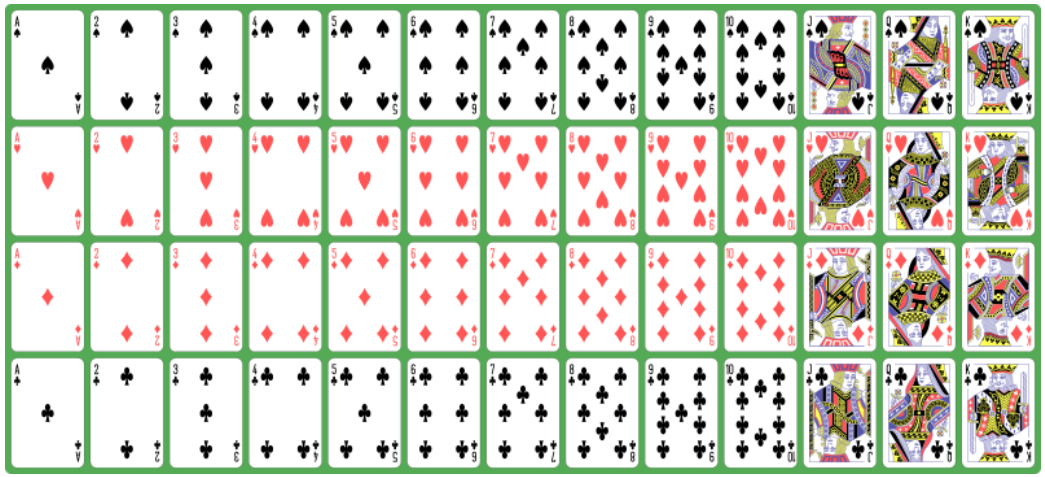
- Start with a standard deck of 52 cards:
  1. Sample a random card:
     (put it back in the deck)
  2. Sample a random card:
     (put it back in the deck)
  3. Sample a random card:
     (put it back in the deck)

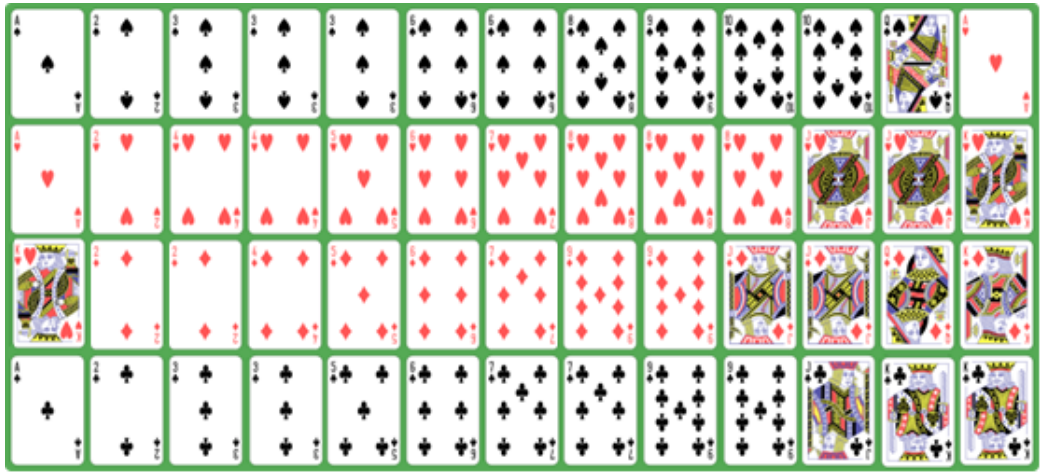
  – …

  52. Sample a random card:
      (which may be a repeat)
- We now have a new deck of 52 cards:





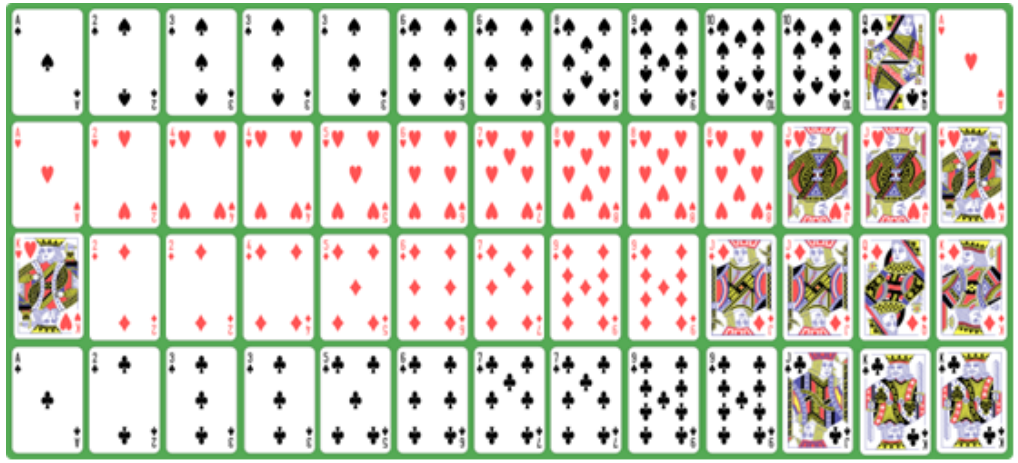




https://commons.wikimedia.org/wiki/File:English_pattern_playing_cards_deck.svg

Bootstrap Sampling

- New 52-card deck is "bootstrap sample":



  - Some cards will be missing, and some cards will be duplicated.
    - So calculations on the bootstrap sample will give different results than original data.
  - However, the bootstrap sample roughly maintains trends:
    - Roughly 25% of the cards will be diamonds.
    - Roughly 3/13 of the cards will be "face" cards.
    - There will be roughly four "10" cards.
  - Common use: compute a statistic based on several bootstrap samples.
    - Gives you an idea of how the statistic varies as you vary the data.

Random Forest Ingredient 1: Bootstrap

- Bootstrap sample of a list of 'n' examples:
  - A new set of size 'n' chosen independently with replacement.

```
for i in 1:n
    j = rand(1:n)   # pick a random number from {1,2,...,n}
    X_bootstrap[i,:] = X[j,:]   # use the random sample
```

  - Gives new dataset of 'n' examples, with some duplicated and some missing.
    - Approximately 63% of original examples will be included for large 'n'.

- Bagging: using bootstrap samples for ensemble learning.
  - Generate several bootstrap samples of the examples (x_i, y_i).
  - Fit a classifier to each bootstrap sample.
  - At test time, average the predictions.

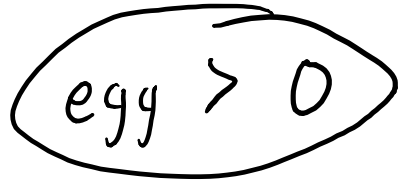
} Decision trees will make different splits.

Random Forest Ingredient 2: Random Trees

- For each split in a random tree model:
  - Randomly sample a small number of possible features (typically $\sqrt{d}$).
  - Only consider these random features when searching for the optimal rule.

Random tree 1:
- sample (milk, oranges)

Random tree 2:
- sample (egg, lactase)



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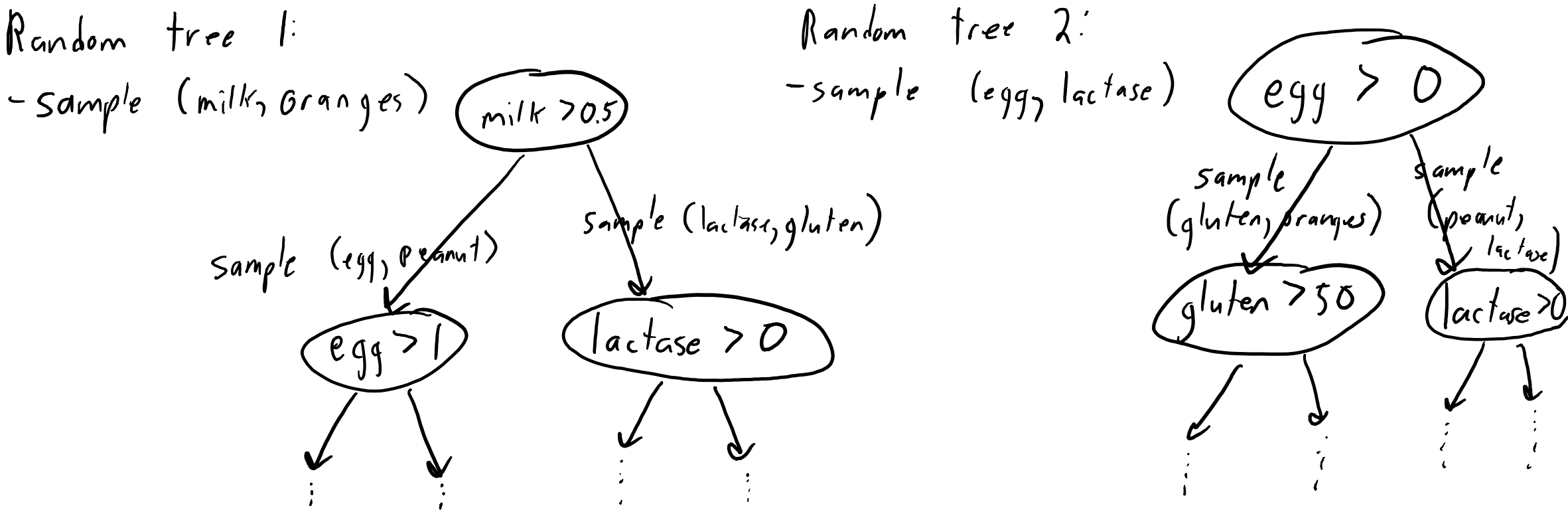

Random Forest Ingredient 2: Random Trees

- For each split in a random tree model:
  - Randomly sample a small number of possible features (typically $\sqrt{d}$).
  - Only consider these random features when searching for the optimal rule.
- Splits will tend to use different features in different trees.
  - They will still overfit, but hopefully errors will be more independent.
- So the average tends to have a much lower test error.
- Empirically, random forests are one of the "best" classifiers.
- Fernandez-Delgado et al. [2014]:
  - Compared 179 classifiers on 121 datasets.
  - Random forests are most likely to be the best classifier.

Summary

- Encouraging invariance:
  - Add transformed data to be insensitive to the transformation.
- Ensemble methods take classifiers as inputs.
  - Try to reduce either E_{train} or E_{approx} without increasing the other much.
  - "Boosting" reduces E_{train} and "averaging" reduces E_{approx}.
- Averaging:
  - Improves predictions of multiple classifiers if errors are independent.
- Random forests:
  - Averaging of deep randomized decision trees.
  - One of the best "out of the box" classifiers.

- Next time:
  - We start unsupervised learning.

Extremely-Randomized Trees

- Extremely-randomized trees add an extra level of randomization:
  1. Each tree is fit to a bootstrap sample.
  2. Each split only considers a random subset of the features.
  3. Each split only considers a random subset of the possible thresholds.

- So instead of considering up to ‘n’ thresholds, only consider 10 or something small.
  - Leads to different partitions so potentially more independence.

Text Example 1: Language Identification

- Consider data that doesn't look like this:

$$X = \begin{bmatrix} 0.5377 & 0.3188 & 3.5784 \\ 1.8339 & -1.3077 & 2.7694 \\ -2.2588 & -0.4336 & -1.3499 \\ 0.8622 & 0.3426 & 3.0349 \end{bmatrix}, \quad y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix},$$

- But instead looks like this:

$$X = \begin{bmatrix} \text{Do you want to go for a drink sometime?} \\ \text{J'achète du pain tous les jours.} \\ \text{Fais ce que tu veux.} \\ \text{There are inner products between sentences?} \end{bmatrix}, y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix}.$$

- How should we represent sentences using features?

A (Bad) Universal Representation

- Treat character in position ‘j’ of the sentence as a categorical feature.
  - “fais ce que tu veux” => x_i = [f a i s ‘’ c e ‘’ q u e ‘’ t u ‘’ v e u x .]
- “Pad” end of the sentence up to maximum #characters:
  - “fais ce que tu veux” => x_i = [f a i s ‘’ c e ‘’ q u e ‘’ t u ‘’ v e u x . γ γ γ γ γ γ γ γ …]
- Advantage:
  - No information is lost, KNN can eventually solve the problem.
- Disadvantage: throws out everything we know about language.
  - Needs to learn that “veux” starting from any position indicates “French”.
    - Doesn’t even use that sentences are made of words (this must be learned).
  - High overfitting risk, you will need a lot of examples for this easy task.

Bag of Words Representation

- Bag of words represents sentences/documents by word counts:

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ICML	International	Conference	Machine	Learning	Leading	Academic
1	2	2	2	2	1	1

- Bag of words loses a ton of information/meaning:
  - But it easily solves language identification problem

Universal Representation vs. Bag of Words

- Why is bag of words better than "string of characters" here?
  - It needs less data because it captures invariances for the task:
    - Most features give strong indication of one language or the other.
    - It doesn't matter *where* the French words appear.
  - It overfits less because it throws away irrelevant information.
    - Exact sequence of words isn't particularly relevant here.

Text Example 2: Word Sense Disambiguation

- Consider the following two sentences:
  - "The cat ran after the mouse."
  - "Move the mouse cursor to the File menu."

- Word sense disambiguation (WSD): classify "meaning" of a word:
  - A surprisingly difficult task.

- You can do ok with bag of words, but it will have problems:
  - "Her mouse clicked on one cat video after another."
  - "We saw the mouse run out from behind the computer."
  - "The mouse was gray." (ambiguous without more context)

Bigrams and Trigrams

- A bigram is an ordered set of two words:
  - Like “computer mouse” or “mouse ran”.
- A trigram is an ordered set of three words:
  - Like “cat and mouse” or “clicked mouse on”.

- These give more context/meaning than bag of words:
  - Includes neighbouring words as well as order of words.
  - Trigrams are widely-used for various language tasks.

- General case is called n-gram.
  - Unfortunately, coupon collecting becomes a problem with larger ‘n’.

Why does Bootstrapping select approximately 63%?

- Probability of an arbitrary x_i being selected in a bootstrap sample:

p(selected at least once in 'n' trials)

$= 1 -$ p(not selected in any of 'n' trials)

$= 1 - ($p(not selected in one trial))^n

$= 1 - (1 - 1/n)^n$

$\approx 1 - 1/e$

≈ 0.63

(trials are independent)

(prob $= \frac{n-1}{n}$ for choosing any of the n-1 other samples)

($(1 - 1/n)^n \to e^{-1}$ as $n \to \infty$)

Why Random Forests Work

- Consider ‘k’ independent classifiers, whose errors have a variance of σ^2.
- If the errors are IID, the variance of the average is σ^2/k.
  - So the more classifiers you average, the more you decrease error variance. (And the more the training error approximates the test error.)
- Generalization to case where classifiers are not independent is:

$$c\sigma^2 + \frac{(1-c)}{k}\sigma^2$$

  - Where ‘c’ is the correlation.
- So the less correlation you have the closer you get to independent case.
- Randomization in random forests decreases correlation between trees.
  - See also “Sensitivity of Independence Assumptions”.

Boosting: Key Ideas

- Input to boosting is classifier that:
  - Is simple enough that it doesn't overfit much.
  - Can obtain >50% weighted training accuracy

- Example: decision stumps or low-depth decision trees.

Boosting: Key Ideas

- Basic steps:
  1. Fit a classifier on the training data.
  2. Give a higher weight to examples that the classifier got wrong.
  3. Fit a classifier on the weighted training data.
  4. Go back to 2.
- Final prediction: weighted vote of individual classifier predictions.
- Boosted decision trees are very fast/accurate classifiers.
  - "AdaBoost": classic boosting method.
  - "XGBoost": recent method that has been winning Kaggle competitions.

How these concepts often show up in practice

- Here is a recent e-mail related to many ideas we've recently covered:
  - "However, the performance did not improve while the model goes deeper and with augmentation. The best result I got on validation set was 80% with LeNet-5 and NO augmentation (LeNet-5 with augmentation I got 79.15%), and later 16 and 50 layer structures both got 70%~75% accuracy.

    In addition, there was a software that can use mathematical equations to extract numerical information for me, so I trained the same dataset with nearly 100 features on random forest with 500 trees. The accuracy was 90% on validation set.

    I really don't understand that how could deep learning perform worse as the number of hidden layers increases, in addition to that I have changed from VGG to ResNet, which are theoretically trained differently. Moreover, why deep learning algorithm cannot surpass machine learning algorithm?"
- Above there is data augmentation, validation error, effect of the fundamental trade-off, the no free lunch theorem, and the effectiveness of random forests.

Bayesian Model Averaging

- Recall the key observation regarding ensemble methods:
  - If models overfit in "different" ways, averaging gives better performance.
- But should all models get equal weight?
  - E.g., decision trees of different depths, when lower depths have low training error.
  - E.g., a random forest where one tree does very well (on validation error) and others do horribly.
  - In science, research may be fraudulent or not based on evidence.
- In these cases, naïve averaging may do worse.

Bayesian Model Averaging

- Suppose we have a set of 'm' probabilistic binary classifiers w_j.
- If each one gets equal weight, then we predict using:

$$p(y_i \mid x_i) = \frac{1}{m} p(y_i \mid w_1, x_i) + \frac{1}{m} p(y_i \mid w_2, x_i) + \cdots + \left(\frac{1}{m}\right) p(y_i \mid w_m, x_i)$$

- Bayesian model averaging treats model 'w_j' as a random variable:

Assume $w_j \perp x_i$

$$p(y_i \mid x_i) = \sum_{j=1}^{m} p(y_i, w_j \mid x_i) = \sum_{j=1}^{m} p(y_i \mid w_j, x_j) p(w_j \mid x_j) = \sum_{j=1}^{m} p(y_i \mid w_j, x_j) p(w_j)$$

- So we should weight by probability that w_j is the correct model:
  - Equal weights assume all models are equally probable.

Bayesian Model Averaging

Again, assuming $w_j \perp X$

- Can get better weights by conditioning on training set:

$$p(w_j \mid X, y) \propto p(y \mid w_j, X)\, p(w_j \mid X) = p(y \mid w_j, X)\, p(w_j)$$

- The 'likelihood' $p(y \mid w_j, X)$ makes sense:
  - We should give more weight to models that predict 'y' well.
  - Note that hidden denominator penalizes complex models.
- The 'prior' $p(w_j)$ is our 'belief' that w_j is the correct model.
- This is how rules of probability say we should weigh models.
  - The 'correct' way to predict given what we know.
  - But it makes some people unhappy because it is subjective.