CPSC 340:
Machine Learning and Data Mining

Ensemble Methods

Fall 2017

Admin

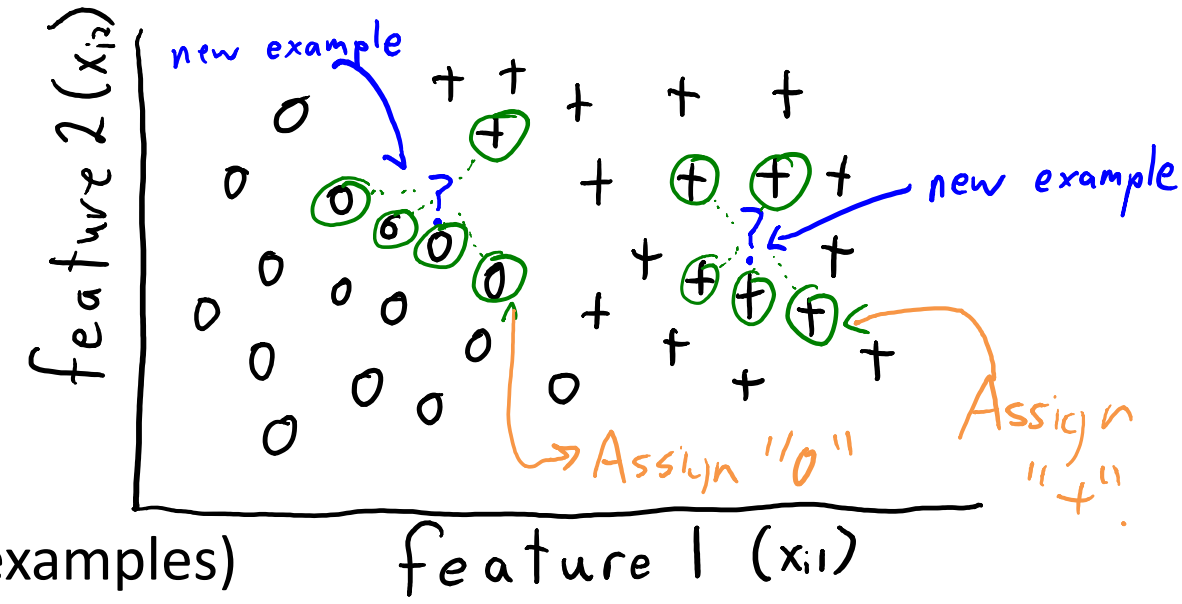
- Welcome to the course!
- Assignment 0:
  - 2 late days to hand it in tonight, 0 after that.
- Assignment 1 is due next Friday.

Last Time: K-Nearest Neighbours (KNN)

- K-nearest neighbours algorithm for classifying ‘x‘:
  - Find ‘k’ values of x_i that are most similar to x.
  - Use mode of corresponding y_i.

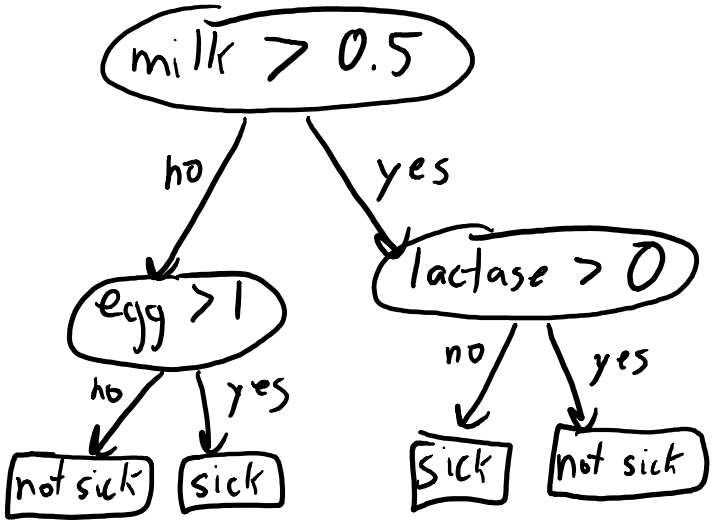
- Lazy learning:
  - To “train” you just store X and y.

- 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

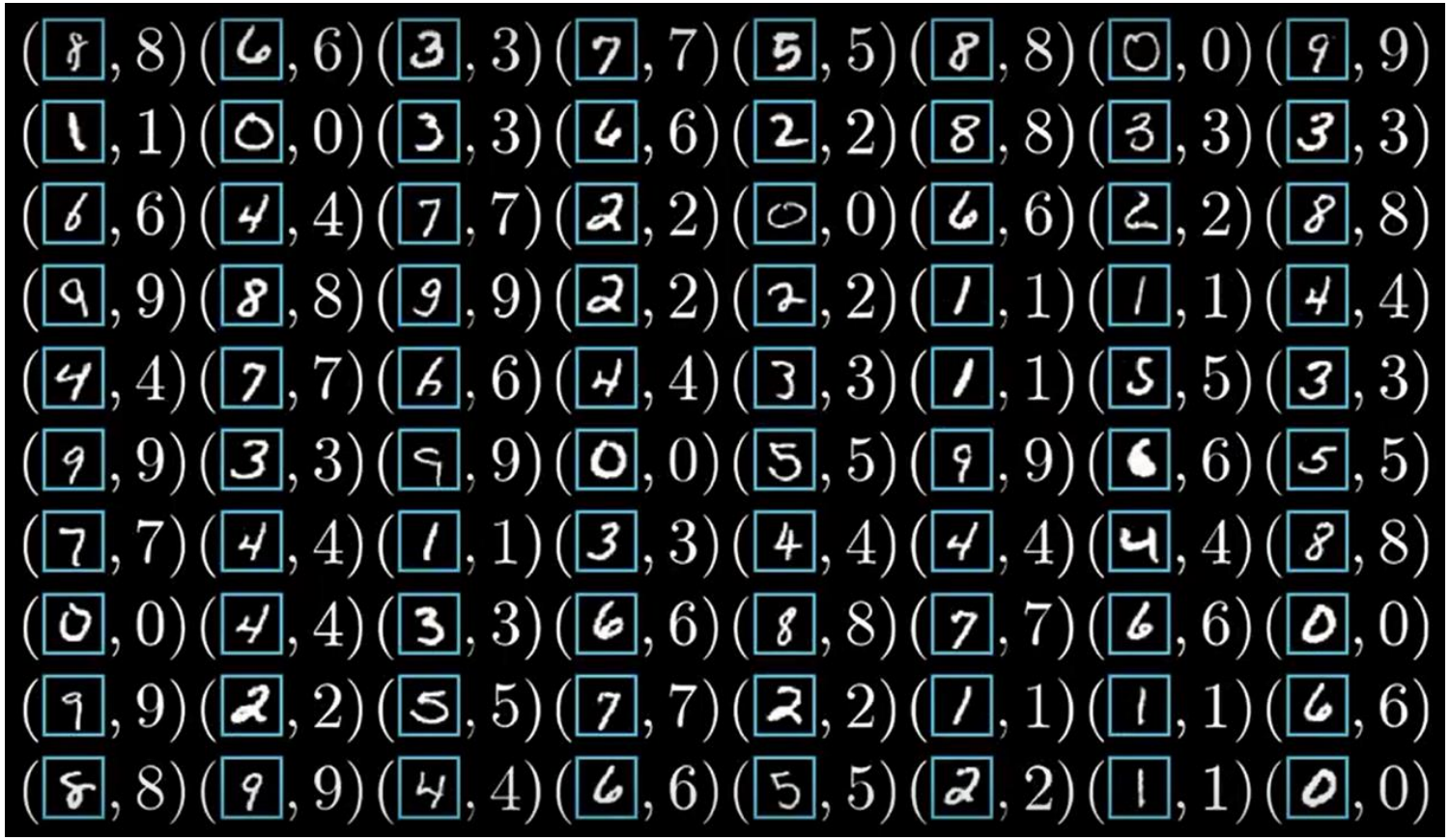


$$p(\text{sick} \mid \text{milk}, \text{egg}, \text{lactase}) \approx p(\text{milk} \mid \text{sick})\, p(\text{egg} \mid \text{sick})\, p(\text{lactase} \mid \text{sick})\, p(\text{sick})$$

(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

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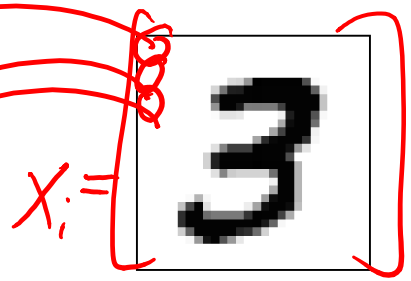


"3"

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

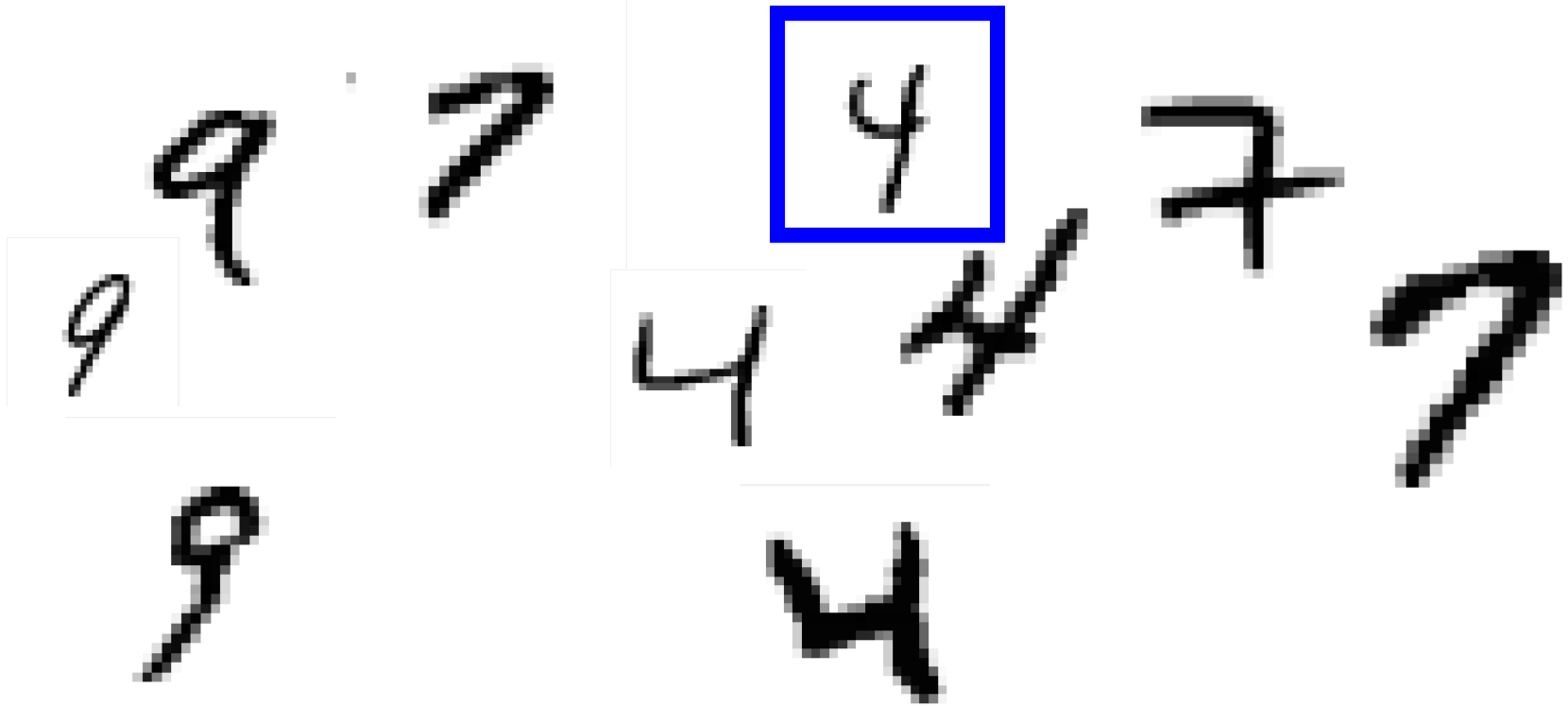
(1,1)	(2,1)	(3,1)	…	(28,1)	(1,2)	(2,2)	…	(14,14)	…	(28,28)
0	0	0		0	0	0		1		0
0	0	0		0	0	0		1		0
0	0	0		0	0	0		0		0
0	0	0		0	0	0		1		0

char
3
6
0
9

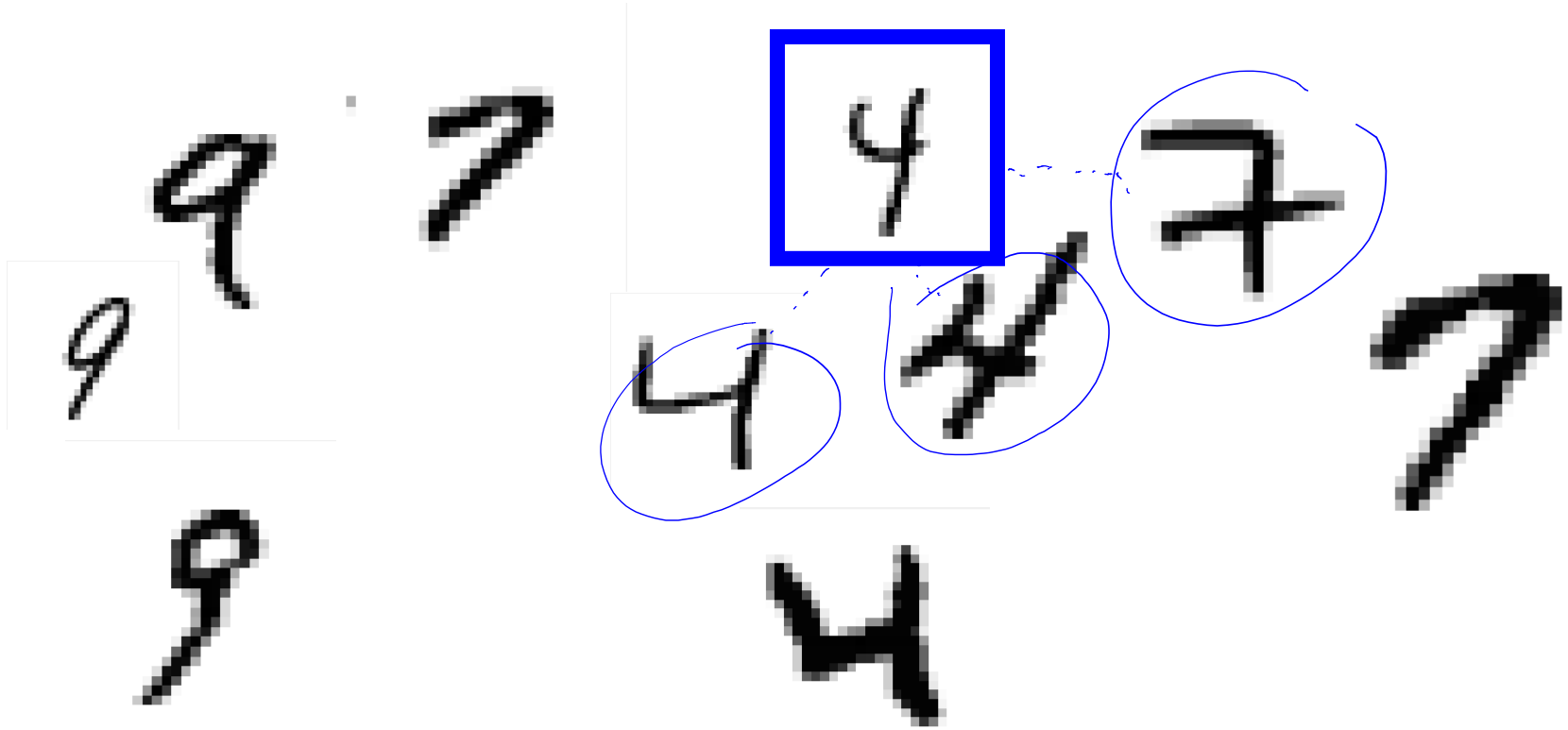
Each feature is grayscale intensity of one of the 784 pixels

KNN for Optical Character Recognition

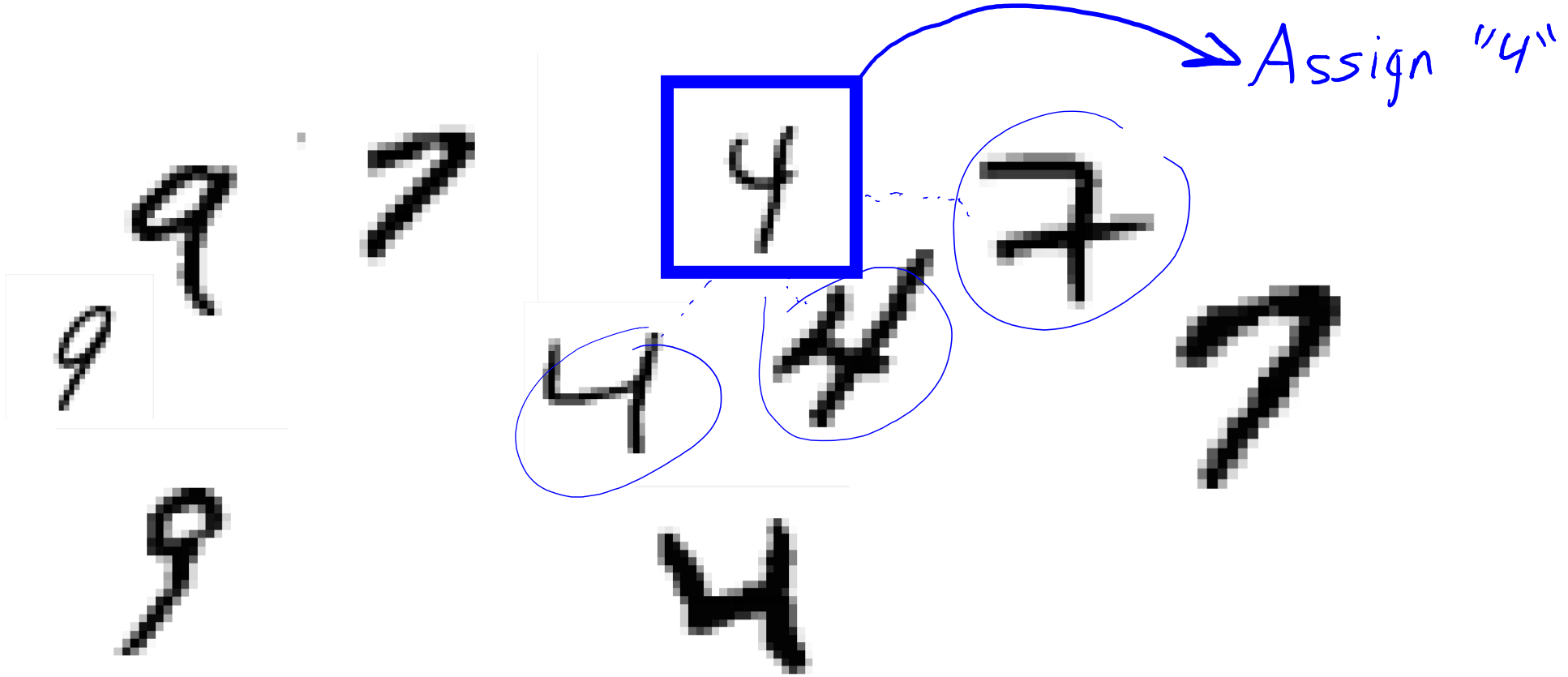
KNN for Optical Character Recognition



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:

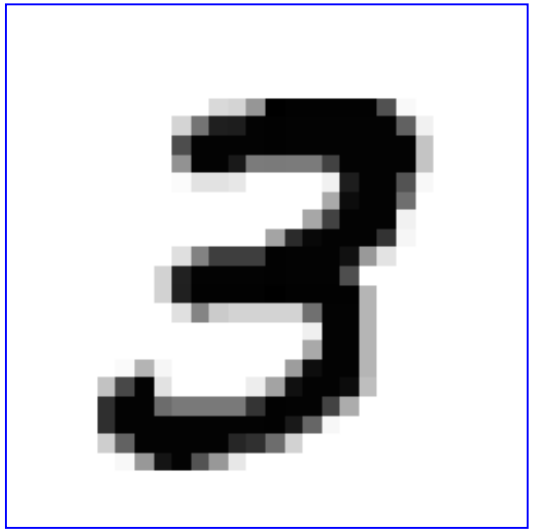
What we see:

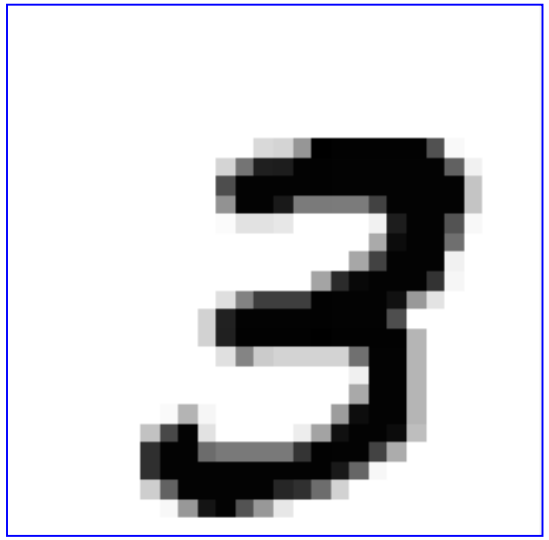
What the computer “sees”:

Actually, it’s worse:

What the Computer Sees

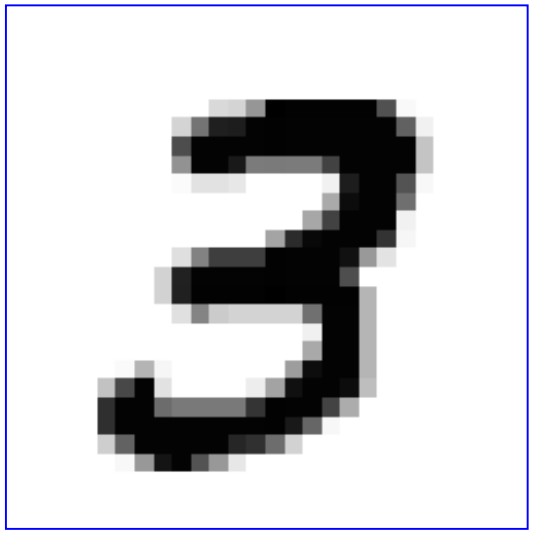
- Are these two images “similar”?

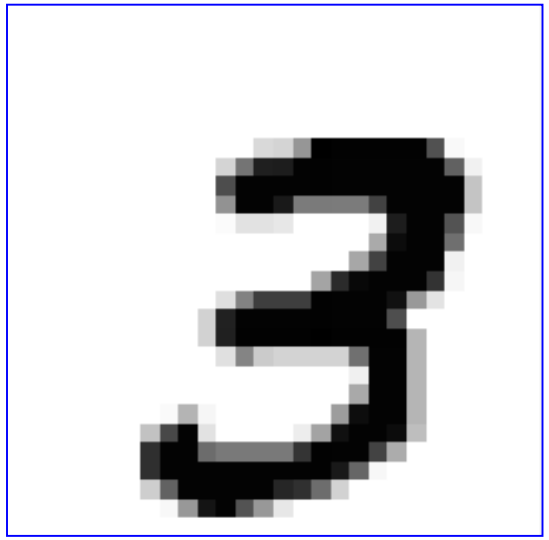




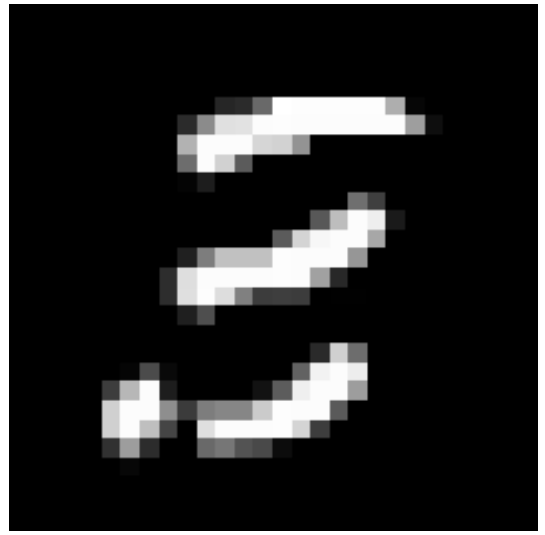
What the Computer Sees

- Are these two images “similar”?





Difference:

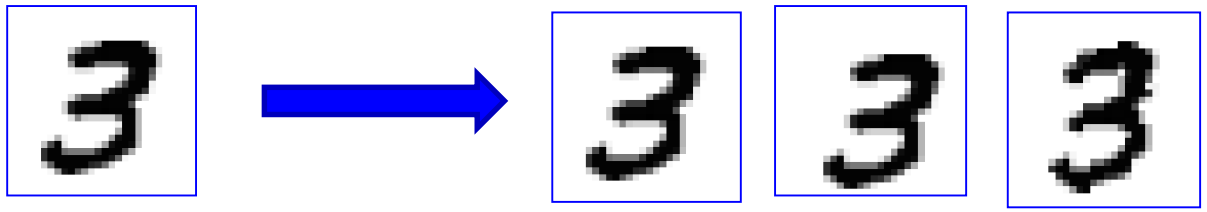


- KNN does not know that labels should be translation invariant.

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.

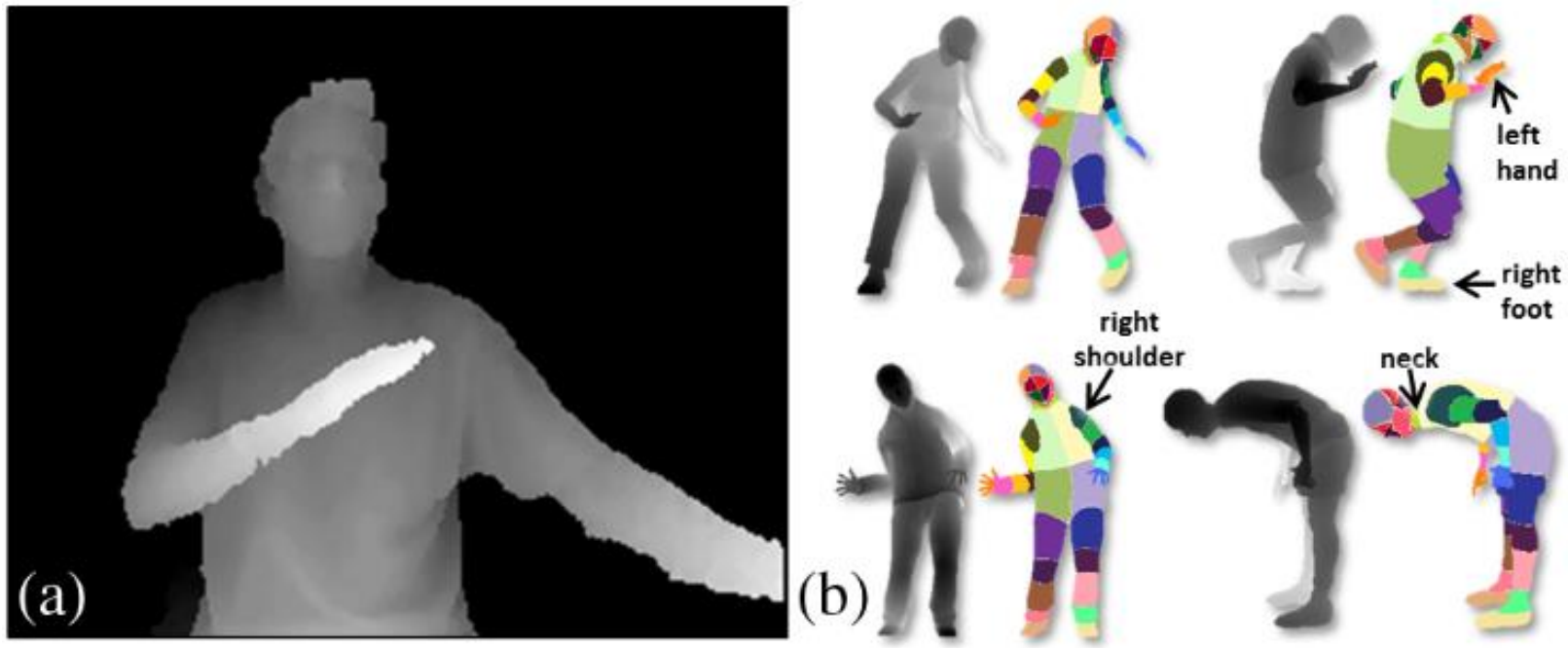
- The easy/fast way is to just add transformed data during training:
  - Add translated/rotate/resized/warped versions of training images.



  - Crucial part of many successful vision systems.
  - Bonus slides discuss invariant features for language data.

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.

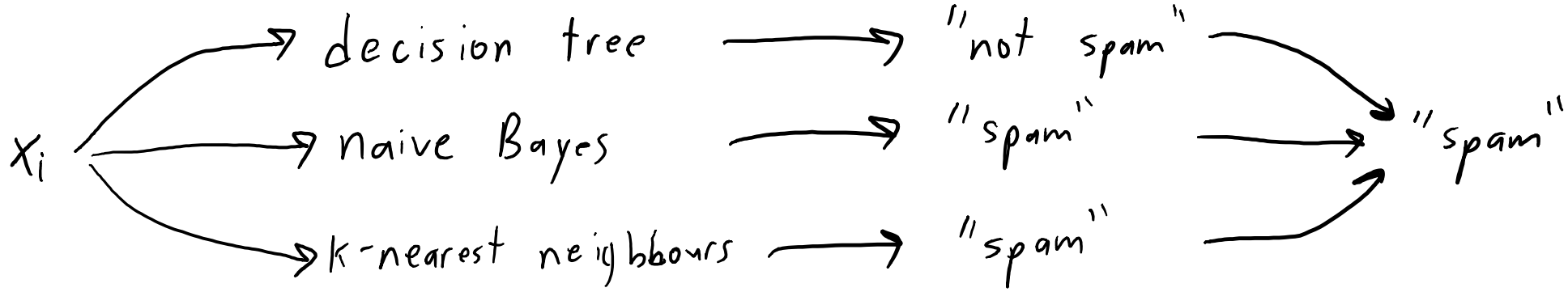
  2. E_{approx}: How well training error approximates the test error.
- Goal of ensemble methods is that meta-classifier:
  - Does much better on one of these than individual classifiers.
  - Doesn't do too much worse on the other.
- This suggests two types of ensemble methods:
  1. Boosting: improves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

Averaging

- 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 all of these are 80% accurate, what should we predict?

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 if probabilistic).



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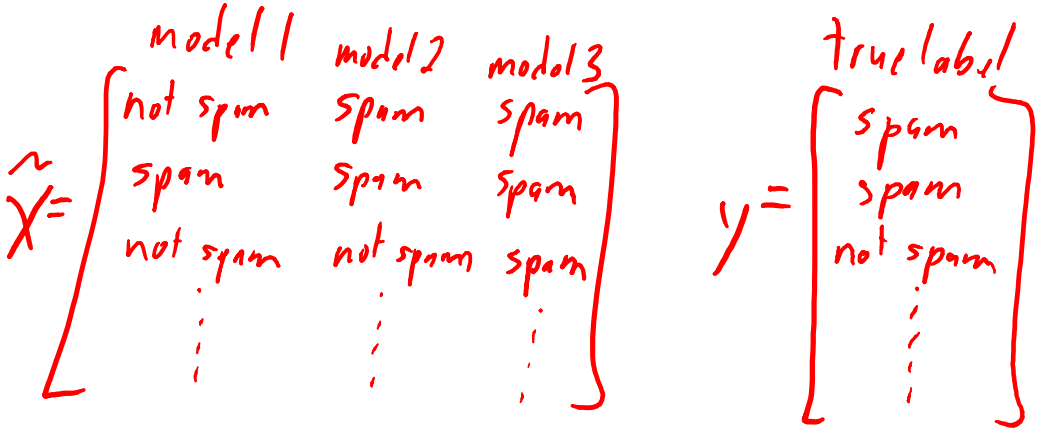
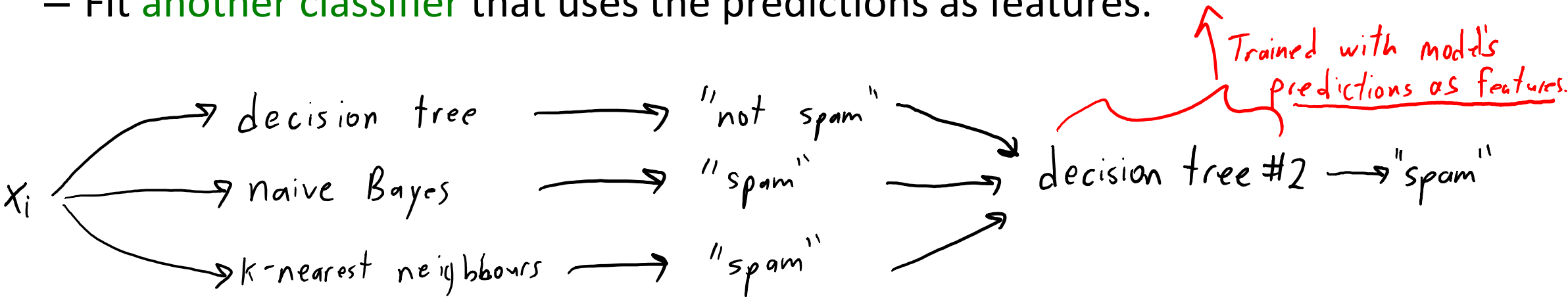


- Stacking:
  - Fit another classifier that uses the predictions as features.



Averaging

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

- Why does this work?
- Consider classifiers that tend to 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.

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.

Random Forest Ingredient 1: Boostrap

- Bootstrap sample of a list of 'n' objects:
  - Another set of 'n' objects, 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' objects, with some duplicated and some missing.
    - Approximately 63% of original objects will be included for large 'n'.
  - Very common in statistics to estimate sensitivity of statistic to data.
- Bagging: using bootstrap samples for ensemble learning.
  - Generate several bootstrap samples of the objects (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

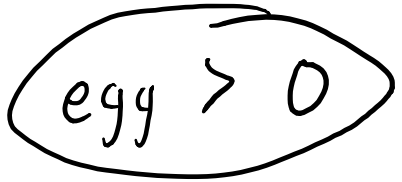
- For each split in a random tree model:
  - Randomly sample a small number of possible features.
  - Only consider these random features when searching for the optimal rule.

Random tree 1:

- sample (milk, oranges)

Random tree 2:

- sample (egg, lactase)



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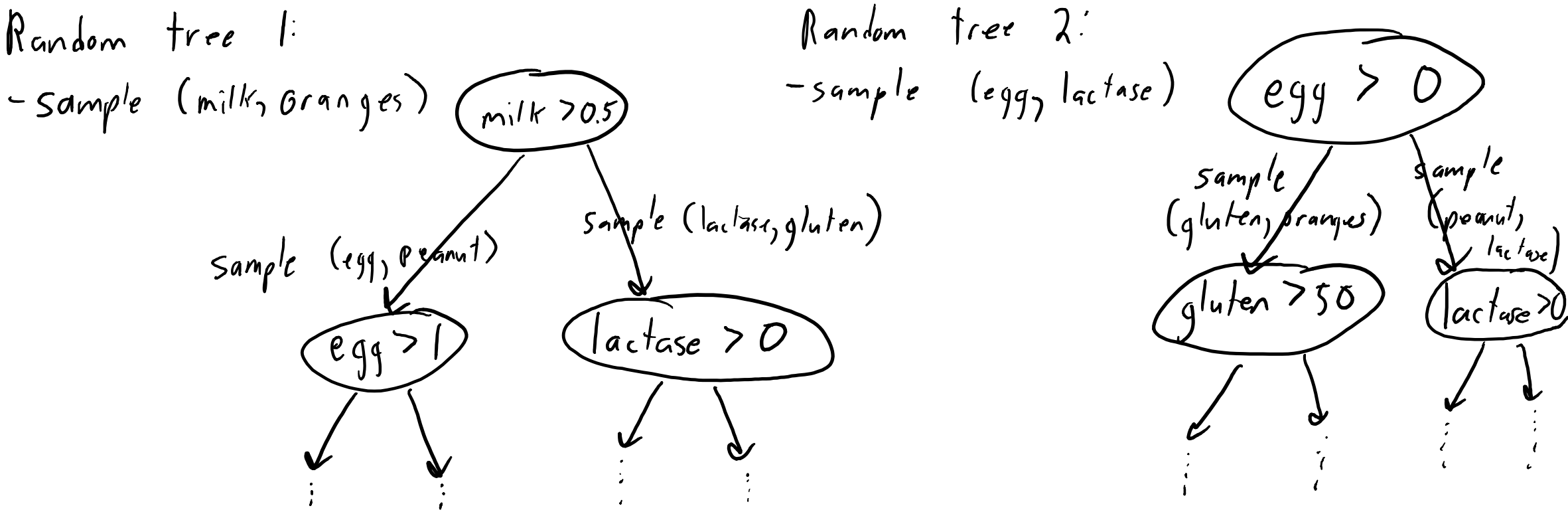

Random Forest Ingredient 2: Random Trees

- For each split in a random tree model:
  - Randomly sample a small number of possible features.
  - 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 make *independent* errors.
- 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.
- 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.

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:

The **International Conference on Machine Learning** (ICML) is the leading international academic conference in machine learning

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’.

Bonus Slide: Why does Bootstrapping give 63%?

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

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

$= 1 - p(\text{not selected in any of 'n' trials})$

$= 1 - (p(\text{not selected in one trial}))^n$

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

$\approx 1 - 1/e$

≈ 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 can Averaging Work?

- Consider having '3' binary classifiers, that are each independently right with probability 0.80:
  - 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.
  - Note that it's important that classifiers are at least somewhat independent, have probability of being right > 0.5, and that the probabilities aren't too different (otherwise, you may be better off just picking the best one).

Bonus Slide: 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.

Bonus Slide: 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.

Bonus Slide: 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.

Bonus Slide: Bayesian Model Averaging

- 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.