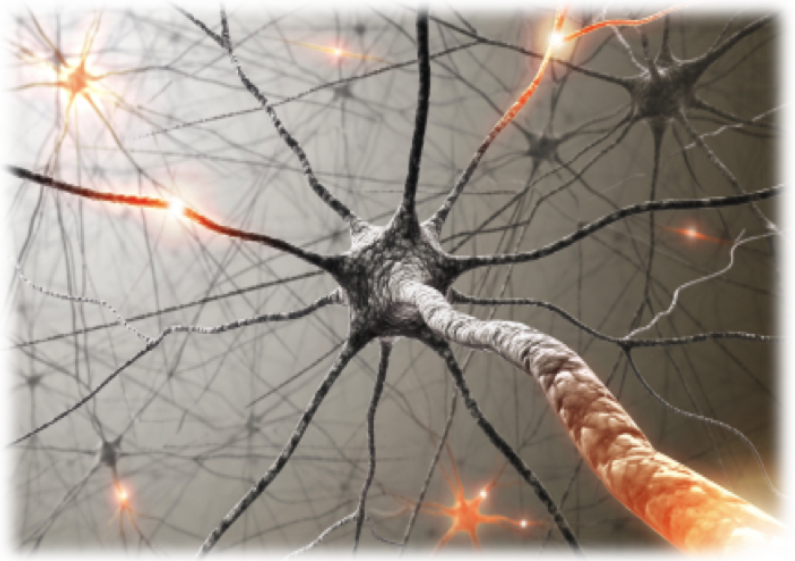
Lecture 4: Machine learning III



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Question

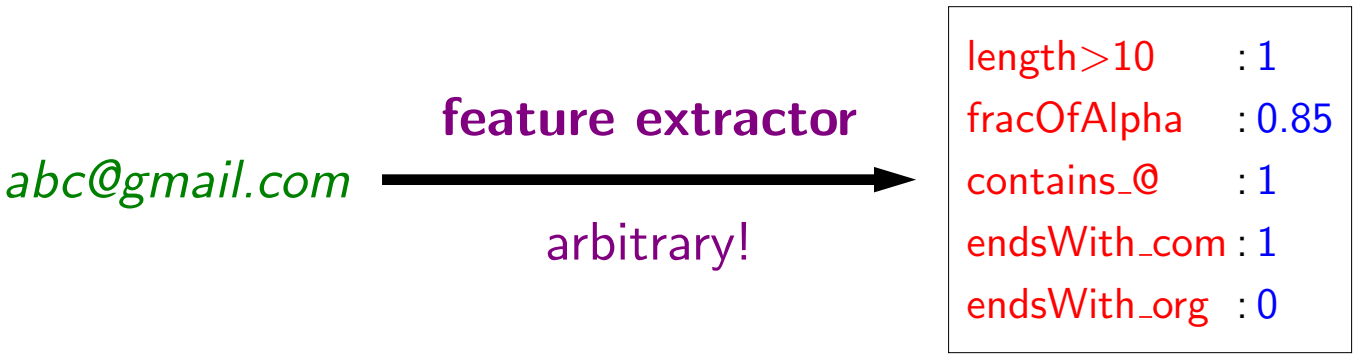
What's the true objective of machine learning?

- minimize error on the training set
- minimize training error + regularizer
- minimize error on unseen future examples
- to learn about machines

- So far in this class, we have tried to cast everything as a well-defined optimization problem. We have even written down an objective function, which is the average loss (error) on the training data.
- But it turns out that that's not really the true goal. That's only what we tell our optimization friends so that there's something concrete and actionable. The true goal is to minimize error on unseen future examples; in other words, we need to **generalize**. As we'll see, this is perhaps the most important aspect of machine learning and statistics — albeit a somewhat elusive one.

Review

Feature extractor $\phi(x)$:



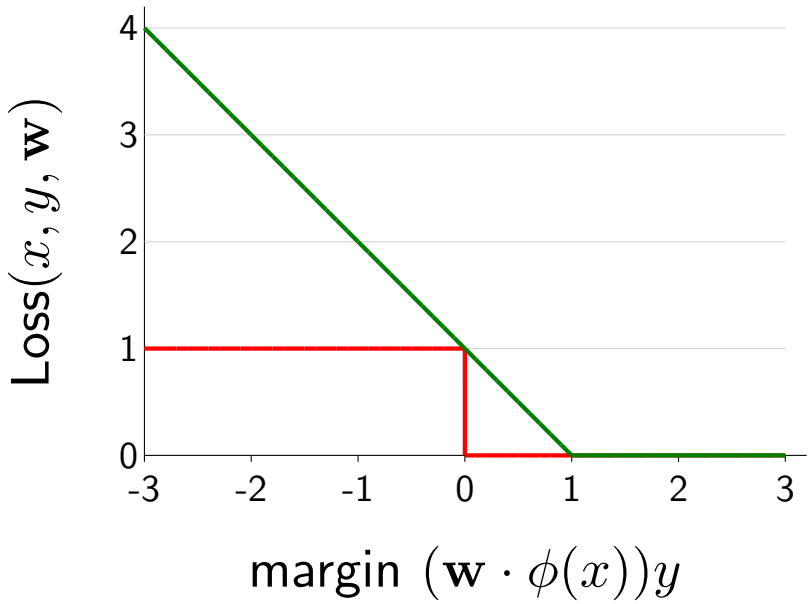
Prediction score:

- Linear predictor: score $= \mathbf{w} \cdot \phi(x)$
- Neural network: score $= \sum_{j=1}^{k} w_j \sigma(\mathbf{v}_j \cdot \phi(x))$

- First a review: last lecture we spoke at length about the importance of features, how to organize them using feature templates, and how we can get interesting non-linearities by choosing $\phi(x)$ judiciously. This is you pouring all your domain knowledge about the problem.
- Given the feature extractor ϕ, we can use that to define a prediction score, either using a linear predictor or a neural network. If you use neural networks, you typically have to work less hard at designing features, but you end up with a harder learning problem. There is a human-machine tradeoff here.

Review

Loss function $\text{Loss}(x, y, \mathbf{w})$:



(for binary classification)

Optimization algorithm: stochastic gradient descent

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{Loss}(x, y, \mathbf{w})$$

- The prediction score is the basis of many types of prediction, including regression and binary classification. The loss function connects the prediction score with the correct output y, and measures how unhappy we are with a particular weight vector $\mathbf{w}$.
- This leads to an optimization problem, that of finding the $\mathbf{w}$ that yields the lowest training loss. We saw that a simple algorithm, stochastic gradient descent, works quite well.

Roadmap

Nearest neighbors

Generalization

Unsupervised learning

Summary

Nearest neighbors

Key idea: similarity

Similar examples tend to have similar outputs.

Algorithm: nearest neighbors

Training: just store $\mathcal{D}_{\text{train}}$

Predictor $f(x')$:

Find $(x, y) \in \mathcal{D}_{\text{train}}$ where $\|\phi(x) - \phi(x')\|$ is smallest

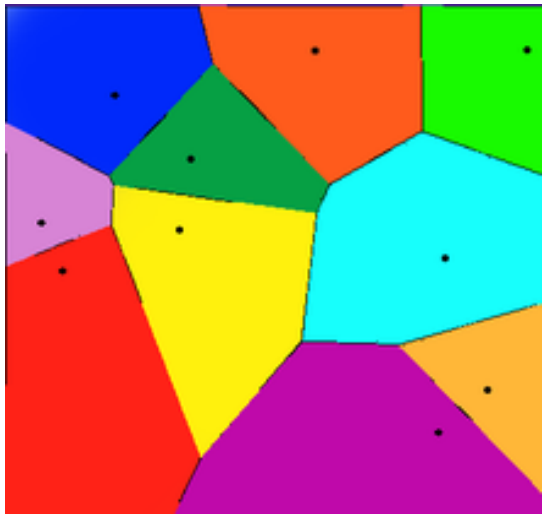
Return y

[demo]

- These slides were skipped last lecture, so we cover them now for completeness.
- **Nearest neighbors** is perhaps conceptually one of the simplest learning algorithms. In a way, there is no learning. At training time, we just store the entire training examples. At prediction time, we get an input x' and we just find the input in our training set that is **most similar**, and return its output.
- In a practical implementation, finding the closest input is non-trivial. Popular choices are using k-d trees or locality-sensitive hashing. We will not worry about this issue.
- The intuition being expressed here is that similar (nearby) points tend to have similar outputs. This is a reasonable assumption in most cases; all else equal, having a body temperature of 37 and 37.1 is probably not going to affect the health prediction by much.

Expressivity of nearest neighbors

Decision boundary: based on Voronoi diagram



- **Non-parametric**: the hypothesis class adapts to number of examples
- Simple and powerful, but kind of brute force

- Let's look at the decision boundary of nearest neighbors. The input space is partitioned into regions, such that each region has the same closest point (this is a Voronoi diagram), and each region could get a different output.
- Notice that this decision boundary is much more expressive than what you could get with quadratic features. In particular, one interesting property is that the complexity of the decision boundary adapts to the number of training examples. As we increase the number of training examples, the number of regions will also increase. Such methods are called **non-parametric**.

Roadmap

Nearest neighbors

Generalization

Unsupervised learning

Summary

Training error

Loss minimization:

$$\arg\min_{\mathbf{w}} \text{TrainLoss}(\mathbf{w})$$

$$\text{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{(x,y) \in \mathcal{D}_{\text{train}}} \text{Loss}(x, y, \mathbf{w})$$

Is this a good objective?

- Now let's be a little more critical about what we've set out to optimize. So far, we've declared that we want to minimize the training loss.

A strawman algorithm

Algorithm: rote learning

Training: just store $\mathcal{D}_{\text{train}}$.

Predictor $f(x)$:

If $(x, y) \in \mathcal{D}_{\text{train}}$: return y.

Else: **segfault**.

Minimizes the objective perfectly (zero), but clearly bad...

- Clearly, machine learning can't be about just minimizing the training loss. The rote learning algorithm does a perfect job of that, and yet is clearly a bad idea. It **overfits** to the training data and doesn't **generalize** to unseen examples.

Evaluation

How good is the predictor f?

Key idea: the real learning objective

Our goal is to minimize **error on unseen future examples**.

Don't have unseen examples; next best thing:

Definition: test set

Test set $\mathcal{D}_{\text{test}}$ contains examples not used for training.

- So what is the true objective then? Taking a step back, what we're doing is building a system which happens to use machine learning, and then we're going to deploy it. What we really care about is how accurate that system is on those **unseen future** inputs.
- Of course, we can't access unseen future examples, so the next best thing is to create a **test set**. As much as possible, we should treat the test set as a pristine thing that's unseen and from the future. We definitely should not tune our predictor based on the test error, because we wouldn't be able to do that on future examples.
- Of course at some point we have to run our algorithm on the test set, but just be aware that each time this is done, the test set becomes less good of an indicator of how well you're actually doing.

Overfitting example 1

Example: overfitting

Input: $x \in \{-4, -3, -2, -1, 1, 2, 3, 4\}$

Output: $y = \text{sign}(x)$, flip 25% of the labels randomly

x	-4	-3	-2	-1	1	2	3	4
y_{train}	-	+	-	-	+	+	+	-
y_{test}	+	-	-	-	+	-	+	+
rote predictions	-	+	-	-	+	+	+	-
linear predictions	-	-	-	-	+	+	+	+

	Train error	Test error	
Rote	0%	50%	— overfits!
Linear	25%	25%	— generalizes!

- To demonstrate overfitting in a simple setting, consider the problem of predicting whether a number x is positive. The data we get is noisy, where 25% of the labels have been flipped randomly.
- If we use rote learning, we will get 0% training error, memorizing the labels. The linear classifier will get 25% error because it mis-classifies the noisy examples.
- However, in the test set, the noise might come in different positions. Now, the rote predictor will get 50% error because it will mis-classify on the inputs where there was noise in the training and in the test. In contrast, the linear classifier is stable and still has 25% error.
- Rote learning **overfits**. The linear predictor **generalizes**.

Another strawman algorithm

Algorithm: majority algorithm

Training: find most frequent output y in $\mathcal{D}_{\text{train}}$.

Predictor $f(x)$: return y.

On the previous example:

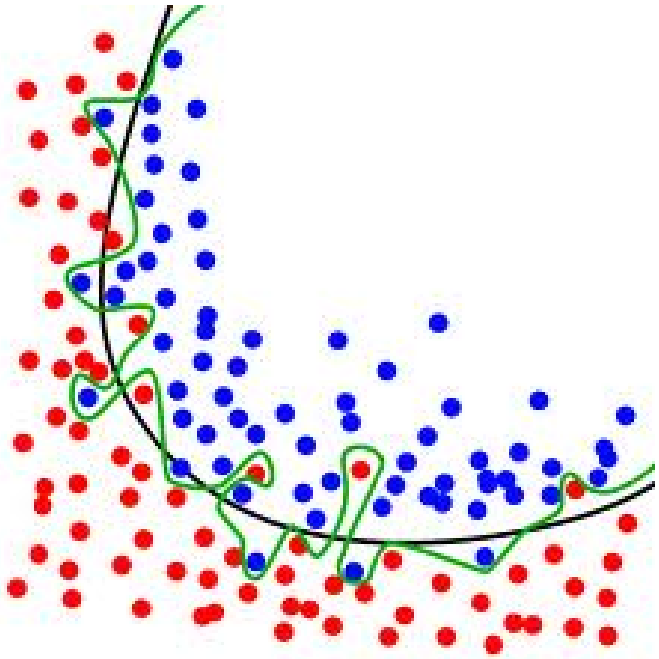
x	-4	-3	-2	-1	1	2	3	4
y_{train}	-	+	-	-	+	+	+	-

	Train error	Test error	
Rote	0%	50%	— overfits!
Linear	25%	25%	— generalizes!
Majority	50%	50%	— generalizes!*

*though the error is high

- It's useful to look at another simple algorithm, which always returns the most frequent output no matter what the input is. Though this algorithm cannot fit the data very well (and thus gets high error rates), it **generalizes** very well.
- Note that strictly speaking, generalization doesn't necessarily mean that you're doing well at test time. It just means that your training error and your test error are not too different.

Overfitting example 2



[demo: compare nearest neighbors and linear classifiers]

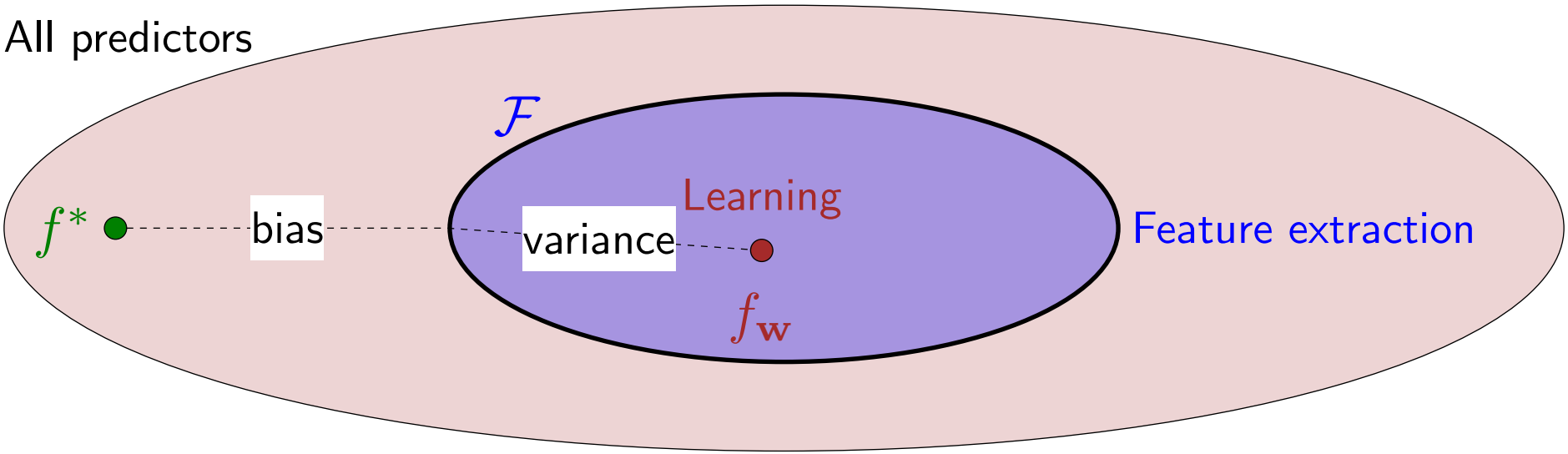
- You might argue that rote learning is obviously a bad idea. Here's a less contrived case of overfitting: comparing nearest neighbors and linear classification. In this demo, nearest neighbors gets zero training error but substantial test error, whereas linear classifiers gets some small error for both. So overfitting leads to worse results, especially when there's noise in our data.

Generalization

When will a learning algorithm **generalize** well?

- So far, we have an intuitive feel for what overfitting is. How do we make this precise? In particular, when does a learning algorithm generalize from the training set to the test set?

Bias and variance

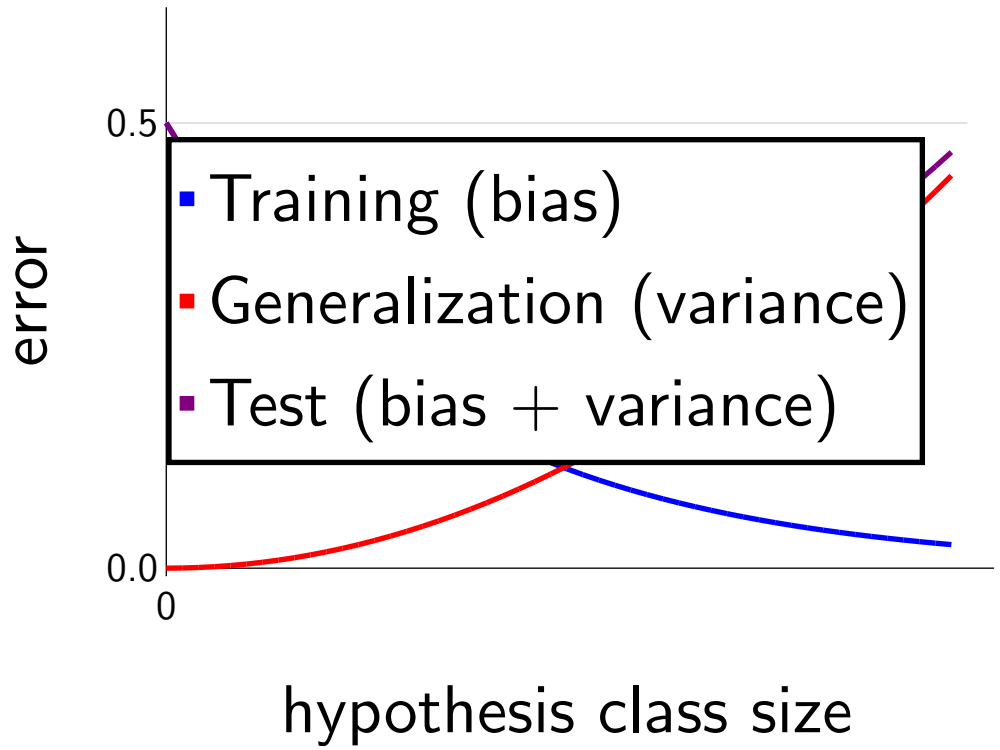


- "Bias": how good is the hypothesis class?
- "Variance": how good is the learned predictor **relative to** the hypothesis class?

Test error is "bias" + "variance"

- Here's a cartoon that can help you understand the balance between fitting and generalization. Out there somewhere, there is a magical predictor f^* that classifies everything perfectly. This predictor is unattainable; all we can hope to do is to use a combination of our domain knowledge and data to approximate that. The question is: how far are we away from f^*?
- Recall that our learning framework consists of (i) choosing a hypothesis class $\mathcal{F}$ (by defining the feature extractor) and then (ii) choosing a particular predictor $f_{\mathbf{w}}$ from $\mathcal{F}$.
- We use the term **bias** to refer to how far the entire hypothesis class is from the target predictor f^*. Larger hypothesis classes have lower bias.
- We use the term **variance** to refer to how good the predictor $f_{\mathbf{w}}$ returned by the learning algorithm is, but only with respect to the hypothesis class. Larger hypothesis classes lead to higher variance because it's harder to know based on limited data which predictor is good.
- We can roughly think about the training error as capturing the bias — how well we can fit. The test error that we care about includes both bias and variance. We'd like both to be small, but there's a tradeoff.
- Note: we are using the terms bias and variance casually here to convey intuition. There is in fact a formal definition of bias and variance, but we will not discuss it here.

Training and test error



Underfitting: bias too high (majority algorithm)

Overfitting: variance too high (rote learning algorithm)

Fitting: balancing bias and variance

- Another way to visualize generalization is by looking at how the various errors vary as a function of the size of the hypothesis class (something we will define more precisely later).
- When the hypothesis class is too small (majority algorithm), then the bias is large, but the variance is small If the hypothesis class is too large (rote learning), then the bias is very small, but the variance is large. The goldilocks hypothesis class is one where we balance bias and variance, and we get a nice fit.

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Question

What are possible ways to reduce overfitting (select all that apply)?

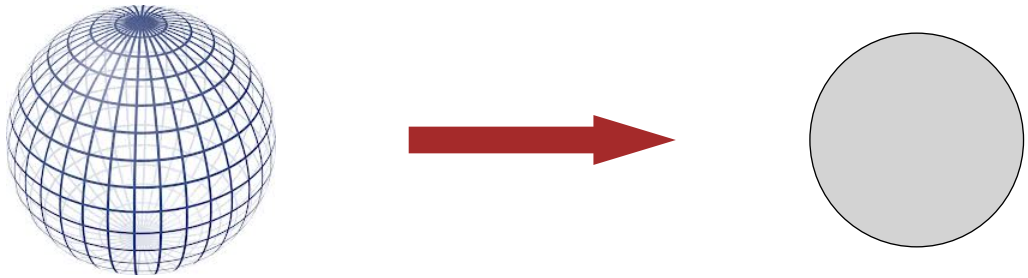
- remove features
- add $0.2\|\mathbf{w}\|^2$ to the objective function
- make sure $\|\mathbf{w}\| \leq 1$
- run SGD for fewer iterations
- round your weights $\mathbf{w}$ to integers

- Now we have seen some concrete examples of overfitting and seen that abstractly, overfitting stems from having too large of a hypothesis class. How do we control the size of the hypothesis class?
- As we will see, all of the options here are valid ways to guard against overfitting.

Controlling size of hypothesis class

Linear predictors are specified by weight vector $\mathbf{w} \in \mathbb{R}^d$

Keeping the dimensionality d small:



Keeping the norm (length) $\|\mathbf{w}\|$ small:

- For each weight vector $\mathbf{w}$, we have a predictor $f_{\mathbf{w}}$ (for classification, $f_{\mathbf{w}}(x) = \mathbf{w} \cdot \phi(x)$). So the hypothesis class $\mathcal{F} = \{f_{\mathbf{w}}\}$ is all the predictors as $\mathbf{w}$ ranges. By controlling the number of possible values of $\mathbf{w}$ that the learning algorithm is allowed to choose from, we control the size of the hypothesis class and thus guard against overfitting.
- There are two ways to do this: keeping the dimensionality d small, and keeping the norm $\|\mathbf{w}\|$ (length of $\mathbf{w}$) small.

Controlling the dimensionality

Manual feature (template) selection:

- Add features if they reduce test error
- Remove features if they don't increase test error

Automatic feature selection (beyond the scope of this class):

- Forward selection
- Boosting
- L_1 regularization

- The most intuitive way to reduce overfitting is to reduce the number of features (or feature templates). Mathematically, you can think about removing a feature $\phi(x)_{37}$ as simply only allowing its corresponding weight to be zero ($w_{37} = 0$).
- Operationally, if you have a few feature templates, then it's probably easier to just manually include or exclude them — this will give you more intuition.
- If you have a lot of individual features, you can apply more automatic methods for selecting features, but these are beyond the scope of this class.

Controlling the norm: regularization

Regularized objective:

$$\min_{\mathbf{w}} \text{TrainLoss}(\mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Algorithm: gradient descent

Initialize $\mathbf{w} = [0, \ldots, 0]$

For $t = 1, \ldots, T$:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta(\nabla_{\mathbf{w}} \text{TrainLoss}(\mathbf{w}) + \lambda\mathbf{w})$$

Same as gradient descent, except shrink the weights towards zero by λ.

Note: SVM = hinge loss + regularization

- A related way to keep the weights small is called **regularization**, which involves adding an additional term to the objective function which penalizes the norm (length) of $\mathbf{w}$. This is probably the most common way to control the norm.
- We can use gradient descent on this regularized objective, and this simply leads to an algorithm which subtracts a scaled down version of $\mathbf{w}$ each iteration. This has the effect of keeping $\mathbf{w}$ closer to the origin than it otherwise would be.

Controlling the norm: early stopping

Algorithm: gradient descent

Initialize $\mathbf{w} = [0, \ldots, 0]$

For $t = 1, \ldots, T$:

$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{TrainLoss}(\mathbf{w})$

Idea: simply make T smaller

Intuition: if have fewer updates, then $\|\mathbf{w}\|$ can't get too big.

Lesson: try to minimize the training error, but don't try too hard.

- A really cheap way to keep the weights small is to do **early stopping**. As we run more iterations of gradient descent, the objective function improves. If we cared about the objective function, this would always be a good thing. However, our true objective is not the training loss.
- Each time we update the weights, $\mathbf{w}$ has the potential of getting larger, so by running gradient descent a fewer number of iterations, we are implicitly ensuring that $\mathbf{w}$ stays small.
- Though early stopping seems hacky, there is actually some theory behind it. And one paradoxical note is that we can sometimes get better solutions by performing less computation.

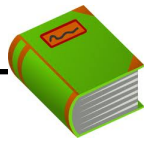
Summary so far

Key idea: keep it simple

Try to minimize training error, but keep the hypothesis class small.

- We've seen several ways to control the size of the hypothesis class (and thus reducing variance) based on either reducing the dimensionality or reducing the norm.
- It is important to note that what matters is the **size** of the hypothesis class, not how "complex" the predictors in the hypothesis class look. To put it another way, using complex features backed by 1000 lines of code doesn't hurt you if there are only 5 of them.
- How the question is: how do we actually decide how big to make the hypothesis class, and in what ways (which features)?

Hyperparameters



Definition: hyperparameters

Properties of the learning algorithm (features, regularization parameter λ, number of iterations T, step size η, etc.).

How do we choose hyperparameters?

Choose hyperparameters to minimize $\mathcal{D}_{\text{train}}$ error? **No** - solution would be to include all features, set $\lambda = 0$, $T \to \infty$.

Choose hyperparameters to minimize $\mathcal{D}_{\text{test}}$ error? **No** - choosing based on $\mathcal{D}_{\text{test}}$ makes it an unreliable estimate of error!

Validation

Problem: can't use test set!

Solution: randomly take out 10-50% of training and use it instead of the test set to estimate test error.

Definition: validation set

A **validation (development) set** is taken out of the training data which acts as a surrogate for the **test set**.

- However, if we make the hypothesis class too small, then the bias gets too big. In practice, how do we decide the appropriate size? Generally, our learning algorithm has multiple **hyperparameters** to set. These hyperparameters cannot be set by the learning algorithm on the training data because we would just choose a degenerate solution and overfit. On the other hand, we can't use the test set either because then we would spoil the test set.
- The solution is to invent something that looks like a test set. There's no other data lying around, so we'll have to steal it from the training set. The resulting set is called the **validation set**.
- With this validation set, now we can simply try out a bunch of different hyperparameters and choose the setting that yields the lowest error on the validation set. Which hyperparameter values should we try? Generally, you should start by getting the right order of magnitude (e.g., $\lambda = 0.0001, 0.001, 0.01, 0.1, 1, 10$) and then refining if necessary.

Development cycle

Problem: simplified named-entity recognition

Input: a string x (e.g., *President Barack Obama in*)

Output: y, whether x is a person or not (e.g., $+1$)

Algorithm: recipe for success

- Split data into train, dev, test
- Look at data to get intuition
- Repeat:
  - Implement feature / tune hyperparameters
  - Run learning algorithm
  - Sanity check train and dev error rates, weights
  - Look at errors to brainstorm improvements
- Run on test set to get final error rates

[live solution]

- This slide represents the most important yet most overlooked part machine learning: how do actually apply it in practice.
- We have so far talked about the mathematical foundation of machine learning (loss functions and optimization), and discussed some of the conceptual issues surrounding overfitting, generalization, size of hypothesis classes. But what actually spend most of your time doing is not writing new algorithms, but going through a **development cycle**, where you iteratively improve your system.
- Suppose you're given a binary classification task (backed by a dataset). What is the process by which you get to a working system? There are many ways to do this; here is one that I've found to be effective
- The key is to stay connected with the data and the model, and have intuition about what's going on. It can be hard sometimes, as machine learning algorithms (even linear classifiers) are often not the easiest things to understand when you have thousands of parameters.
- First, maintain data hygiene. Hold out a test set from your data that you don't look at until you're done. Start by looking at the data to get intuition. You can start to brainstorm what features / predictors you will need. You can compute some basic statistics.
- Then you enter a loop: implement a new feature. There are three things to look at: error rates, weights, and predictions. First, sanity check the error rates and weights to make sure you don't have an obvious bug. Then do an **error analysis** to see which examples your predictor are actually getting wrong. The art of practical machine learning is turning these observations into new features.
- Finally, run your system once on the test set and report the number you get. If your test error is much higher than your development error, then you probably did too much tweaking and were **overfitting** (at a meta-level) the development set.

Roadmap

Nearest neighbors

Generalization

Unsupervised learning

Summary

Supervision?

Supervised learning:

- Prediction: $\mathcal{D}_{\text{train}}$ contains input-output pairs (x, y)
- Fully-labeled data is very **expensive** to obtain (we can get 10,000 labeled examples)

Unsupervised learning:

- Clustering: $\mathcal{D}_{\text{train}}$ only contains inputs x
- Unlabeled data is much **cheaper** to obtain (we can get 100 million unlabeled examples)

- We have so far covered the basics of **supervised learning**. If you get a labeled training set of (x, y) pairs, then you can train a predictor. However, where do these examples (x, y) come from? If you're doing image classification, someone has to sit down and label each image, and generally this tends to be expensive enough that we can't get that many examples.
- On the other hand, there are tons of **unlabeled examples** sitting around (e.g., Flickr for photos, Wikipedia, news articles for text documents). The main question is whether we can harness all that unlabeled data to help us make better predictions? This is the goal of **unsupervised learning**.

[Brown et al, 1992]

Word clustering using HMMs

Input: raw text (100 million words of news articles)...

Output:

Cluster 1: Friday Monday Thursday Wednesday Tuesday Saturday Sunday weekends Sundays Saturdays
Cluster 2: June March July April January December October November September August
Cluster 3: water gas coal liquid acid sand carbon steam shale iron
Cluster 4: great big vast sudden mere sheer gigantic lifelong scant colossal
Cluster 5: man woman boy girl lawyer doctor guy farmer teacher citizen
Cluster 6: American Indian European Japanese German African Catholic Israeli Italian Arab
Cluster 7: pressure temperature permeability density porosity stress velocity viscosity gravity tension
Cluster 8: mother wife father son husband brother daughter sister boss uncle
Cluster 9: machine device controller processor CPU printer spindle subsystem compiler plotter
Cluster 10: John George James Bob Robert Paul William Jim David Mike
Cluster 11: anyone someone anybody somebody
Cluster 12: feet miles pounds degrees inches barrels tons acres meters bytes
Cluster 13: director chief professor commissioner commander treasurer founder superintendent dean custodian
Cluster 14: had hadn't hath would've could've should've must've might've
Cluster 15: head body hands eyes voice arm seat eye hair mouth

Impact: used in many state-of-the-art NLP systems

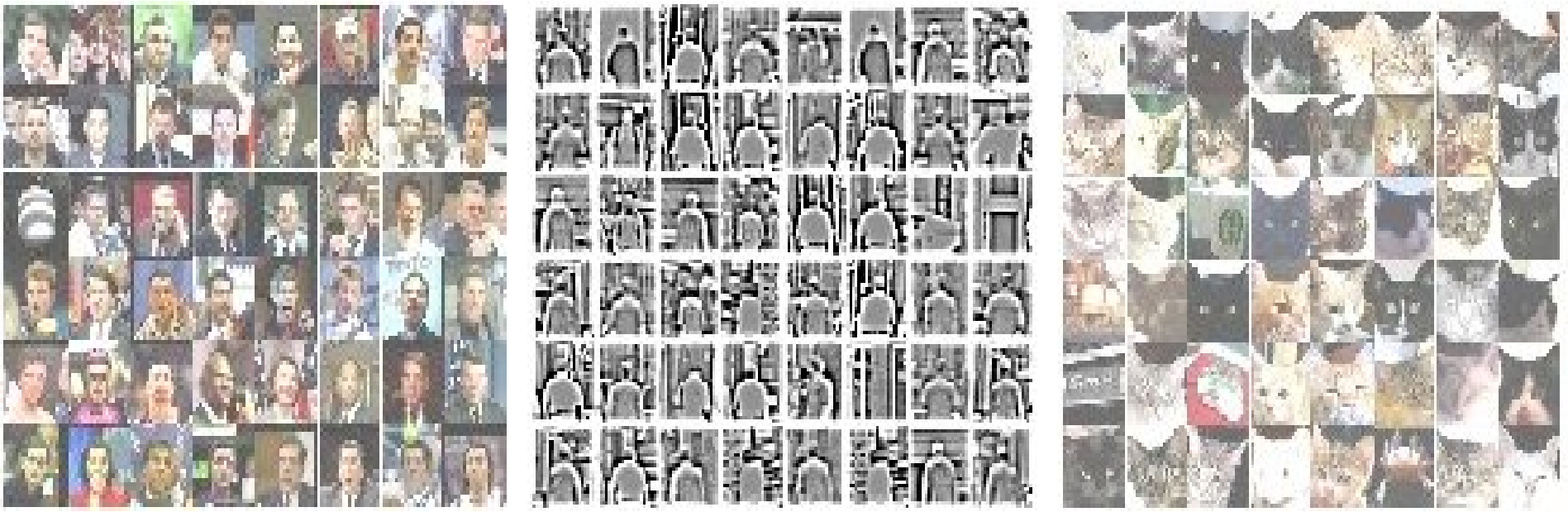
- Empirically, unsupervised learning has produced some pretty impressive results. HMMs can be used to take a ton of raw text and clusters related words together.

[Le et al, 2012]

Feature learning using neural networks

Input: 10 million images (sampled frames from YouTube)

Output:



Impact: state-of-the-art results on object recognition (22,000 categories)

- An unsupervised variant of neural networks called autoencoders can be used to take a ton of raw images and output clusters of images. No one told the learning algorithms explicitly what the clusters should look like — they just figured it out.

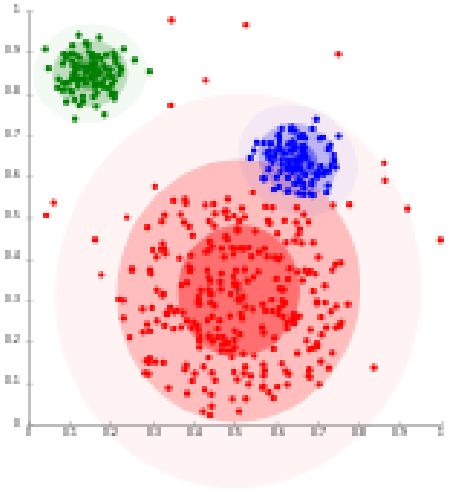
Key idea: unsupervised learning

Data has lots of rich **latent** structures; want methods to discover this **structure** automatically.

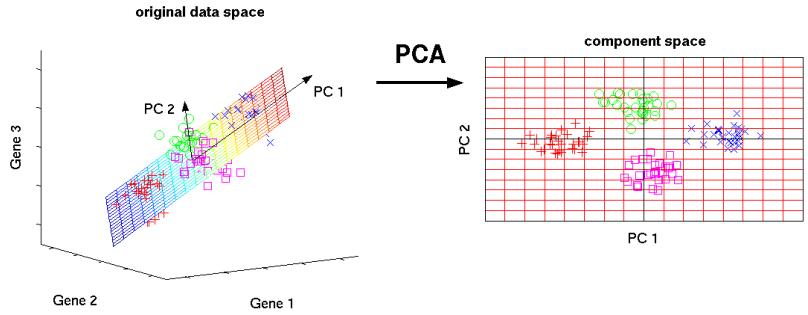
- Unsupervised learning in some sense is the holy grail: you don't have to tell the machine anything — it just "figures it out." However, one must not be overly optimistic here: there is no free lunch. You ultimately still have to tell the algorithm something, at least in the way you define the features or set up the optimization problem.

Types of unsupervised learning

Clustering (e.g., K-means):

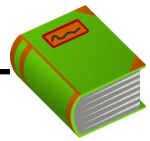


Dimensionality reduction (e.g., PCA):



- There are many forms of unsupervised learning, corresponding to different types of latent structures you want to pull out of your data. In this class, we will focus on one of them: clustering.

Clustering



Definition: clustering

Input: training set of input points

$$\mathcal{D}_{\text{train}} = \{x_1, \ldots, x_n\}$$

Output: assignment of each point to a cluster

$$[z_1, \ldots, z_n] \text{ where } z_i \in \{1, \ldots, K\}$$

Intuition: Want similar points to be put in same cluster, dissimilar points to put in different clusters

[whiteboard]

- The task of clustering is to take a set of points as input and return a partitioning of the points into K clusters. We will represent the partitioning using an **assignment vector** $z = [z_1, \ldots, z_n]$; for each i, $z_i \in \{1, \ldots, K\}$ specifies which of the K clusters point i is assigned to.

K-means objective

Setup:

- Each cluster $k = 1, \ldots, K$ is represented by a **centroid** $\mu_k \in \mathbb{R}^d$
- Intuition: want each point $\phi(x_i)$ close to its assigned centroid μ_{z_i}

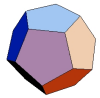
Objective function:

$$\text{Loss}_{\text{kmeans}}(z, \mu) = \sum_{i=1}^{n} \|\phi(x_i) - \mu_{z_i}\|^2$$

Need to choose centroids μ and assignments z **jointly**

- K-means is a particular method for performing clustering which is based on associating each cluster with a **centroid** μ_k for $k = 1, \ldots, K$. The intuition is to assign the points to clusters **and** place the centroid for each cluster so that each point $\phi(x_i)$ is close to its assigned centroid μ_{z_i}.

K-means: simple example



Example: one-dimensional

Input: $\mathcal{D}_{\text{train}} = \{0, 2, 10, 12\}$

Output: $K = 2$ centroids $\mu_1, \mu_2 \in \mathbb{R}$

If know centroids $\mu_1 = 1$, $\mu_2 = 11$:

$$z_1 = \arg\min\{(0-1)^2, (0-11)^2\} = 1$$
$$z_2 = \arg\min\{(2-1)^2, (2-11)^2\} = 1$$
$$z_3 = \arg\min\{(10-1)^2, (12-11)^2\} = 2$$
$$z_4 = \arg\min\{(10-1)^2, (12-11)^2\} = 2$$

If know assignments $z_1 = z_2 = 1$, $z_3 = z_4 = 2$:

$$\mu_1 = \arg\min_\mu (0-\mu)^2 + (2-\mu)^2 = 1$$
$$\mu_2 = \arg\min_\mu (10-\mu)^2 + (12-\mu)^2 = 11$$

- How do we solve this optimization problem? We can't quite just use gradient descent because there are discrete variables (assignment variables z_i). We can't really use dynamic programming because there are continuous variables (the centroids μ_k).
- To motivate the solution, consider a simple example with four points. As always, let's try to break up the problem into subproblems.
- What if we knew the optimal centroids? Then computing the assignment vectors is trivial (for each point, choose the closest center).
- What if we knew the optimal assignments? Then computing the centroids is also trivial (one can check that this is just averaging the points assigned to that center).
- The only problem is that we don't know the optimal centroids or assignments, and unlike in dynamic programming, the two depend on one another cyclically.

K-means algorithm

$$\min_{z} \min_{\mu} \text{Loss}_{\text{kmeans}}(z, \mu)$$

Key idea: alternating minimization

Tackle hard problem by solving two easy problems.

- And now the leap of faith is this: start with an arbitrary setting of the centroids (not optimal). Then alternate between choosing the best assignments given the centroids, and choosing the best centroids given the assignments. This is the K-means algorithm.

K-means algorithm (Step 1)

Goal: given centroids $\mu_1, \ldots, \mu_K$, assign each point to the best centroid.

Algorithm: Step 1 of K-means

For each point $i = 1, \ldots, n$:

Assign i to cluster with closest centroid:

$$z_i \leftarrow \arg\min_{k=1,\ldots,K} \|\phi(x_i) - \mu_k\|^2.$$

- Step 1 of K-means fixes the centroids. Then we can optimize the K-means objective with respect to z alone quite easily. It is easy to show that the best label for z_i is the cluster k that minimizes the distance to the centroid μ_k (which is fixed).

K-means algorithm (Step 2)

Goal: given cluster assignments $z_1, \ldots, z_n$, find the best centroids $\mu_1, \ldots, \mu_K$.

Algorithm: Step 2 of K-means

For each cluster $k = 1, \ldots, K$:

Set μ_k to average of points assigned to cluster k:

$$\mu_k \leftarrow \frac{1}{|\{i : z_i = k\}|} \sum_{i:z_i=k} \phi(x_i)$$

- Now, turning things around, let's suppose we knew what the assignments z were. We can again look at the K-means objective function and try to optimize it with respect to the centroids μ. The best μ_k is to place the centroid at the average of all the points assigned to cluster k.

K-means algorithm

Objective:

$$\min_{z} \min_{\mu} \text{Loss}_{\text{kmeans}}(z, \mu)$$

Algorithm: K-means

Initialize $\mu_1, \ldots, \mu_K$ randomly.

For $t = 1, \ldots, T$:

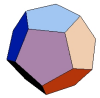
Step 1: set assignments z given μ

Step 2: set centroids μ given z

[demo]

- Now we have the two ingredients to state the full K-means algorithm. We start by initializing all the centroids randomly. Then, we iteratively alternate back and forth between steps 1 and 2, optimizing z given μ and vice-versa.

K-means: simple example



Example: one-dimensional

Input: $\mathcal{D}_{\text{train}} = \{0, 2, 10, 12\}$

Output: $K = 2$ centroids $\mu_1, \mu_2 \in \mathbb{R}$

Initialization (random): $\mu_1 = 0, \mu_2 = 2$

Iteration 1:

- Step 1: $z_1 = 1, z_2 = 2, z_3 = 2, z_4 = 2$
- Step 2: $\mu_1 = 0, \mu_2 = 8$

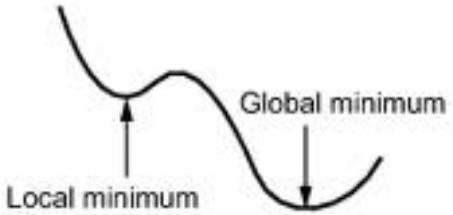
Iteration 2:

- Step 1: $z_1 = 1, z_2 = 1, z_3 = 2, z_4 = 2$
- Step 2: $\mu_1 = 1, \mu_2 = 11$

- Here is an example of an execution of K-means where we converged to the correct answer.

Local minima

K-means is guaranteed to converge to a local minimum, but is not guaranteed to find the global minimum.



[demo: getting stuck in local optima, seed $= 100$]

Solutions:

- Run multiple times from different random initializations
- Initialize with a heuristic (K-means++)

[live solution]

- K-means is guaranteed to decrease the loss function each iteration and will converge to a local minimum, but it is not guaranteed to find the global minimum, so one must exercise caution when applying K-means.
- One solution is to simply run K-means several times from multiple random initializations and then choose the solution that has the lowest loss.
- Or we could try to be smarter in how we initialize K-means. K-means++ is an initialization scheme, which places the centroids on the training points in a way that they tend to be far apart from each other.

Unsupervised learning summary

- Leverage tons of unlabeled data

- Difficult optimization:

latent variables z  parameters μ

Roadmap

Nearest neighbors

Generalization

Unsupervised learning

Summary

Summary

- Feature extraction (think hypothesis classes) [modeling]
- Prediction (linear, neural network, k-means) [modeling]
- Loss functions (compute gradients) [modeling]
- Optimization (stochastic gradient, alternating minimization) [algorithms]
- Generalization (think development cycle) [modeling]

- This concludes our tour of the foundations of machine learning, although machine learning will come up again later in the course. You should have gotten more than just a few isolated equations and algorithms. It is really important to think about the overarching principles in a modular way.
- First, feature extraction is where you put your domain knowledge into. In designing features, it's useful to think in terms of the induced **hypothesis classes** — what kind of functions can your learning algorithm potentially learn?
- These features then drive prediction: either linearly or through a neural network. We can even think of k-means as trying to predict the data points using the centroids.
- Loss functions connect predictions with the actual training examples.
- Note that all of the design decisions up to this point are about modeling. Algorithms are very important, but only come in once we have the right optimization problem to solve.
- Finally, machine learning requires a leap of faith. How does optimizing anything at training time help you generalize to new unseen examples at test time? Learning can only work when there's a common core that cuts past all the idiosyncrasies of the examples. This is exactly what features are meant to capture.

A brief history

1795: Gauss proposed least squares (astronomy)

1940s: logistic regression (statistics)

1952: Arthur Samuel built program that learned to play checkers (AI)

1957: Rosenblatt invented Perceptron algorithm (like SGD)

1969: Minsky and Papert "killed" machine learning

1980s: neural networks (backpropagation, from 1960s)

1990: interface with optimization/statistics, SVMs

2000s-: structured prediction, revival of neural networks, etc.

- Many of the ideas surrounding fitting functions was known in other fields long before computers, let alone AI.
- When computers arrived on the scene, learning was definitely on people's radar, although this was detached from the theoretical statistical and optimization foundations.
- In 1969, Minsky and Papert wrote a famous paper *Perceptrons*, which showed the limitations of linear classifiers with the famous XOR example (similar to our car collision example), which killed off this type of research. AI largely turned to rule-based and symbolic methods.
- Since the 1980s, machine learning has increased its role in AI, been placed on a more solid mathematical foundation with its connection with optimization and statistics.
- While there is a lot of optimism today about the potential of machine learning, there are still a lot of unsolved problems.

Machine learning

Key idea: learning

Programs should improve with experience.

So far: reflex-based models

Next time: state-based models

- If we generalize for a moment, machine learning is really about programs that can improve with experience.
- So far, we have only focused on reflex-based models where the program only outputs a yes/no or a number, and the experience is examples of input-output pairs.
- Next time, we will start looking at models which can perform higher-level reasoning, but machine learning will remain our companion for the remainder of the class.

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Question

What was the most confusing part of today's lecture?