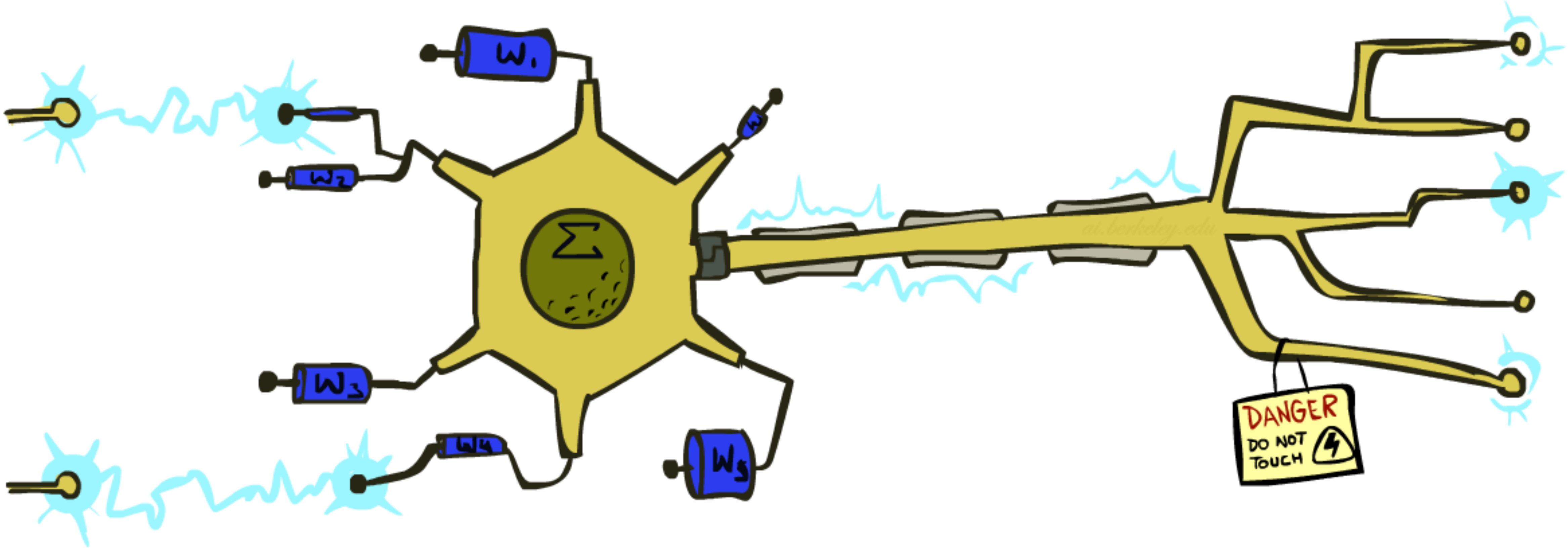
Announcements

- HW8 (HMMs) is due tonight
- HW9 (Perceptrons) has been released. It is due on Thursday Nov 29. Note unusual due date (Thursday rather than Tuesday).
- Midterm 3 will be an in-class exam on the last day of class (Thursday Dec 6).

- Would you like an extra credit homework assignment?

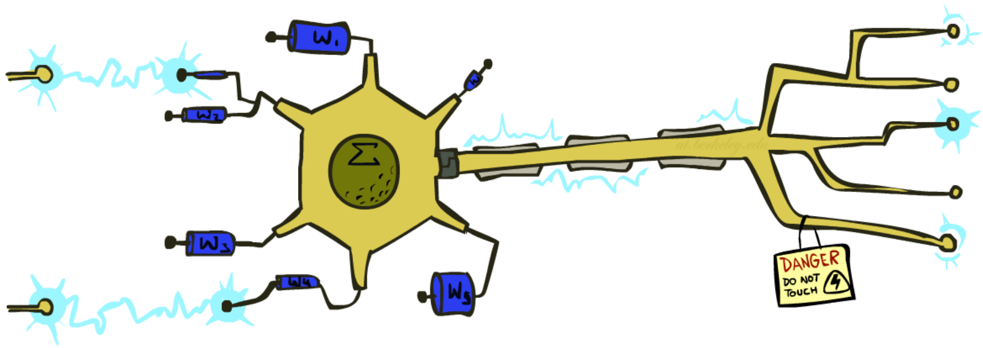
Perceptrons – wrap up



Slides Courtesy of Dan Klein and Pieter Abbeel --- University of California, Berkeley

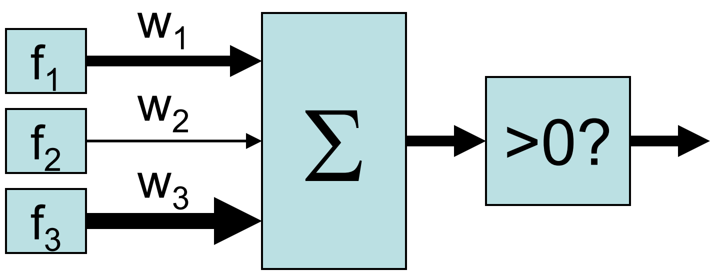
Review: Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

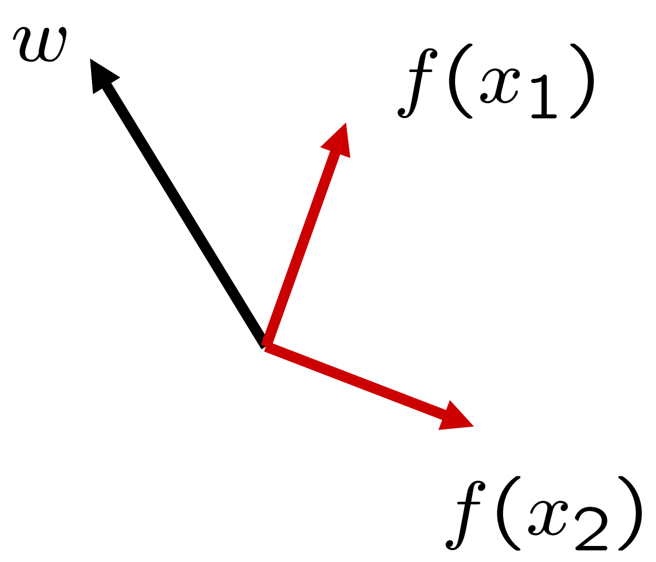
- If the activation is:
  - Positive, output +1
  - Negative, output -1



Review: Weights

- Binary case: compare features to a weight vector
- Learning: figure out the weight vector from examples

```
# free        : 4
YOUR_NAME     :-1
MISSPELLED    : 1
FROM_FRIEND   :-3
...
```




```
# free        : 2
YOUR_NAME     : 0
MISSPELLED    : 2
FROM_FRIEND   : 0
...
```

```
# free        : 0
YOUR_NAME     : 1
MISSPELLED    : 1
FROM_FRIEND   : 1
...
```

Dot product $w \cdot f$ *positive means the positive class*

Review: Decision Rule

- If we have multiple classes:
  - A weight vector for each class:

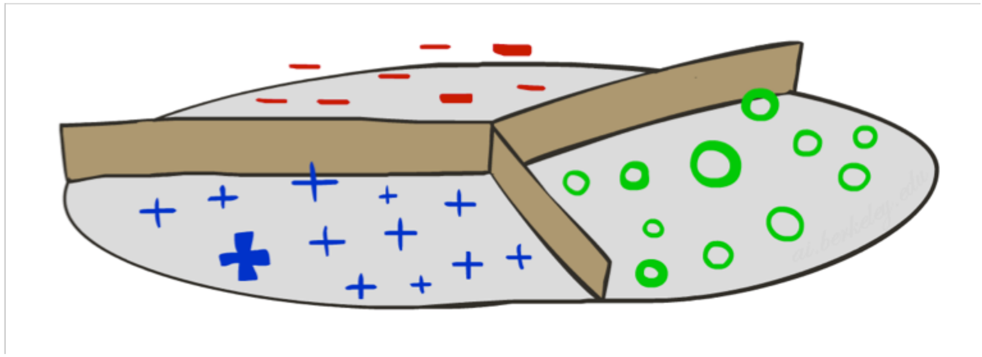
$$w_y$$

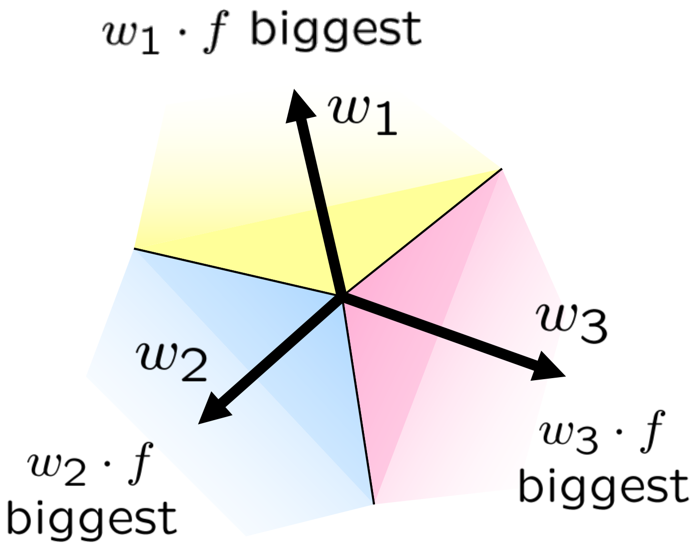
  - Score (activation) of a class y:

$$w_y \cdot f(x)$$

  - Prediction highest score wins

$$y = \arg\max_y \; w_y \cdot f(x)$$





Binary = multiclass where the negative class has weight zero

Review: Multiclass Perceptron

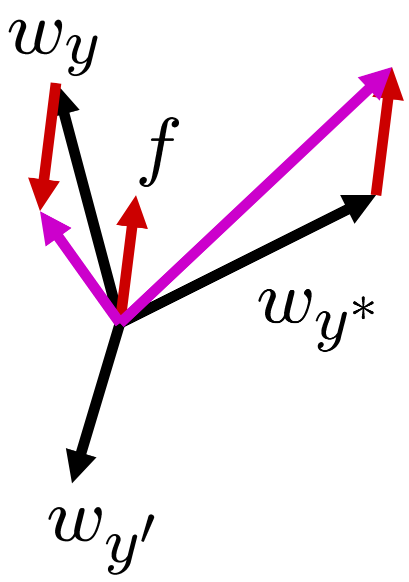
- Start with all weights = 0
- Pick up training examples one by one
- Predict with current weights

$$y = \arg\max_y \; w_y \cdot f(x)$$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

$$w_y = w_y - f(x)$$

$$w_{y^*} = w_{y^*} + f(x)$$



Example: Multiclass Perceptron

"win the vote"

"win the election"

"win the game"

w_{SPORTS}

```
BIAS  : 1
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

$w_{POLITICS}$

```
BIAS  : 0
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

w_{TECH}

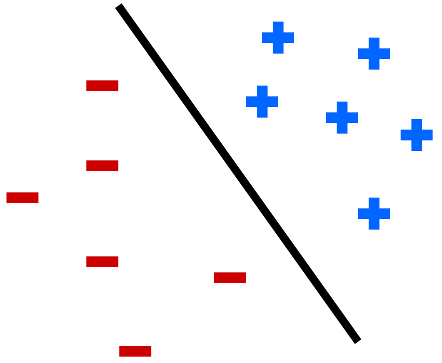
```
BIAS  : 0
win   : 0
game  : 0
vote  : 0
the   : 0
...
```

Properties of Perceptrons

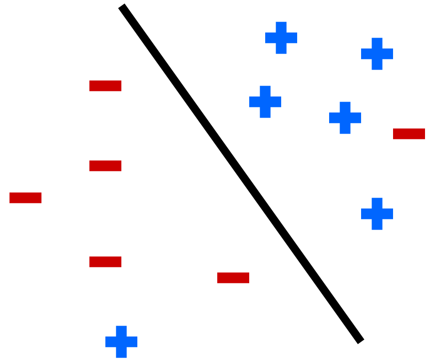
- Separability: true if some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)
- Mistake Bound: the maximum number of mistakes (binary case) related to the *margin* or degree of separability

$$\text{mistakes} < \frac{k}{\delta^2}$$

Separable

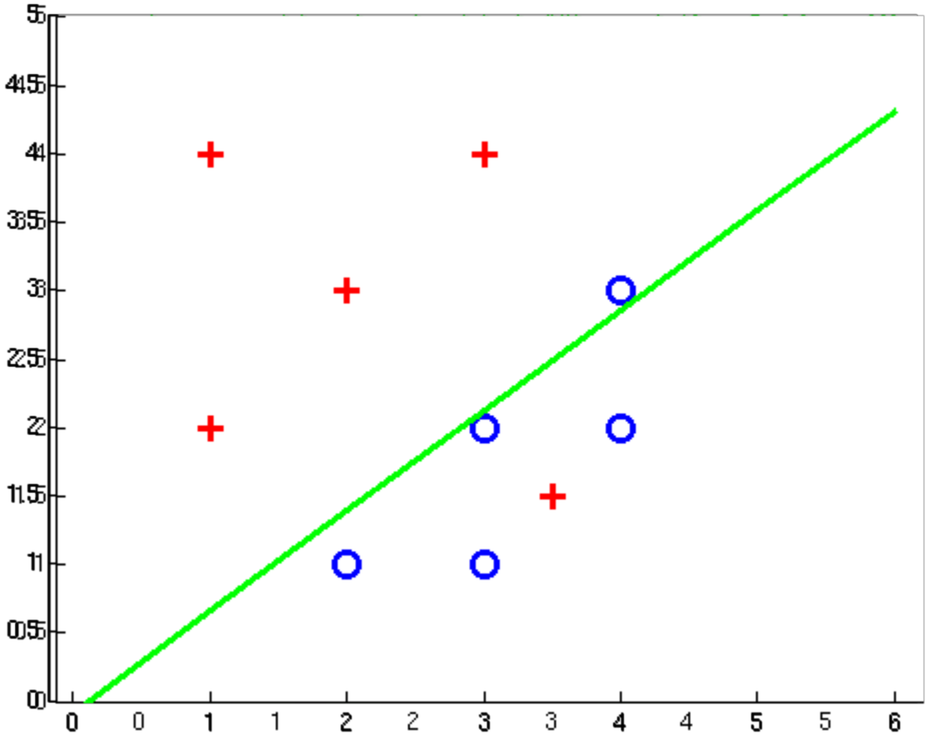


Non-Separable

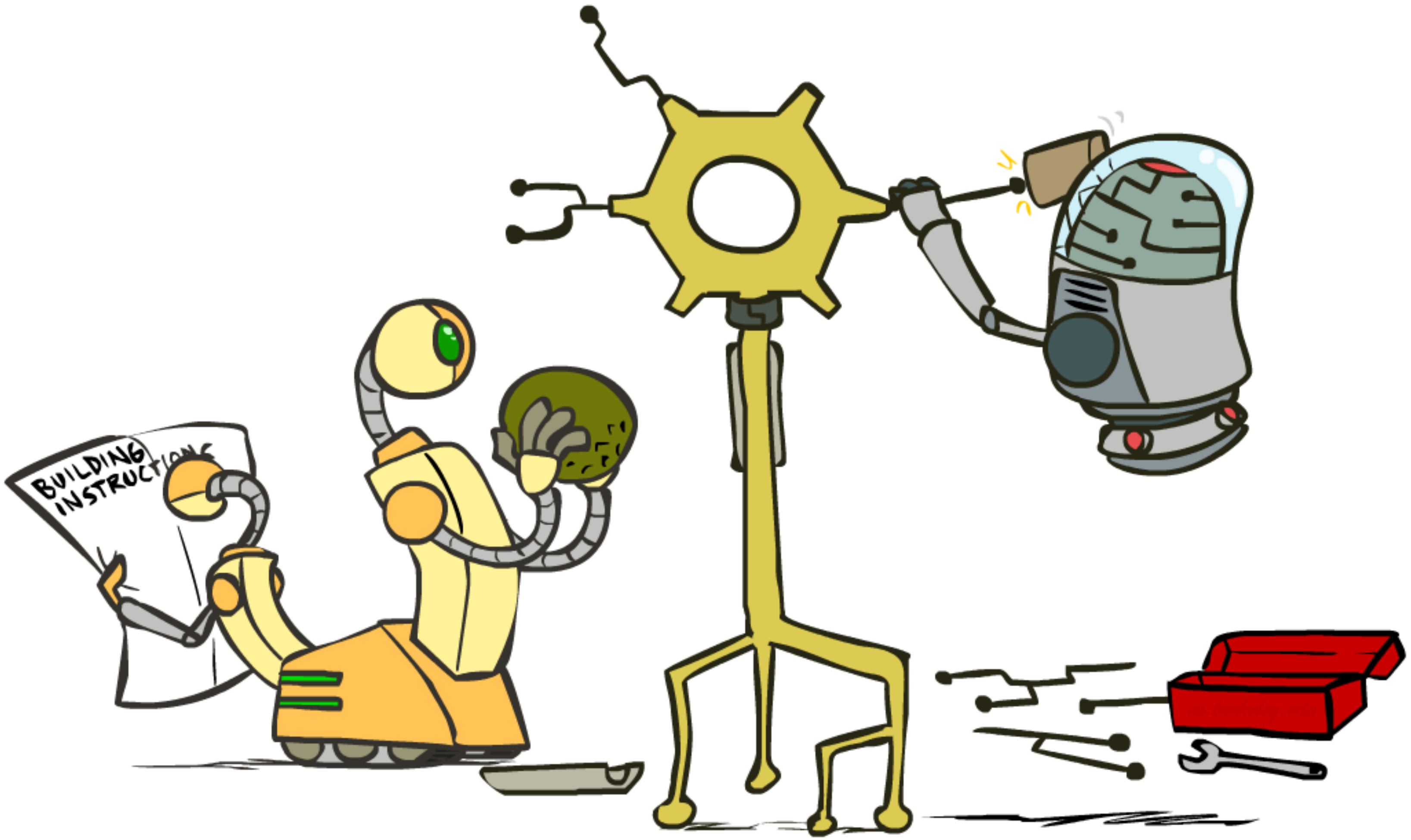


Examples: Perceptron

- Non-Separable Case

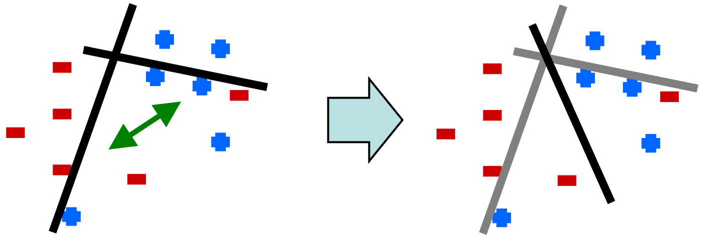


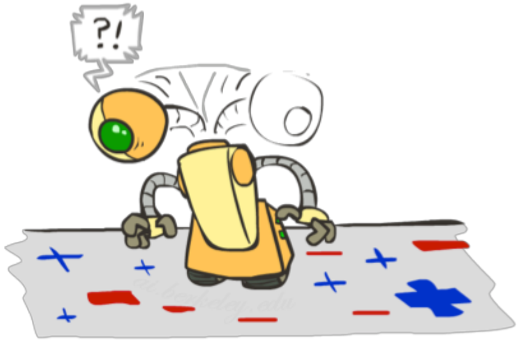
Improving the Perceptron



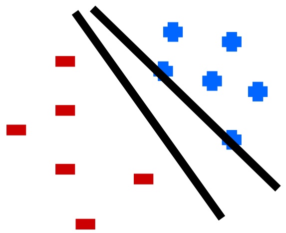
Problems with the Perceptron

- Noise: if the data isn't separable, weights might thrash
  - Averaging weight vectors over time can help (averaged perceptron)

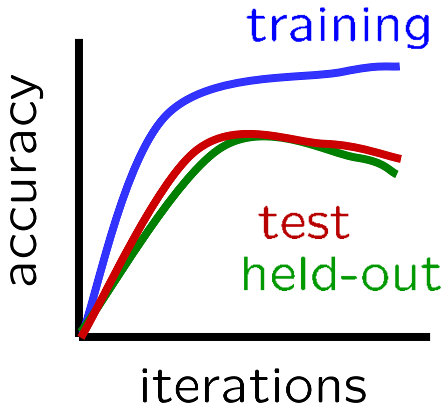


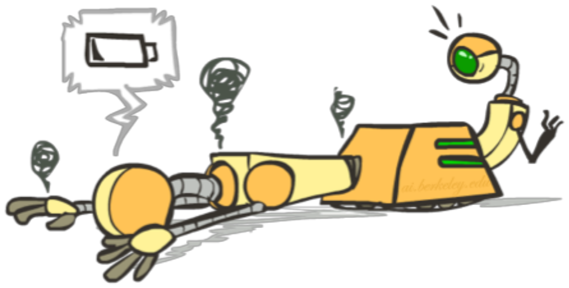


- Mediocre generalization: finds a "barely" separating solution



- Overtraining: test / held-out accuracy usually rises, then falls
  - Overtraining is a kind of overfitting





Fixing the Perceptron

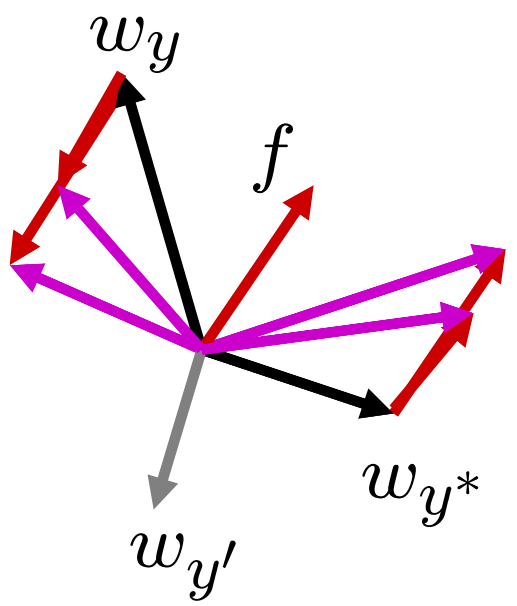
- Idea: adjust the weight update to mitigate these effects

- MIRA*: choose an update size that fixes the current mistake…
- … but, minimizes the change to w

$$w_{y^*} \cdot f(x) \geq w_y \cdot f(x) + 1$$

- The +1 helps to generalize

* Margin Infused Relaxed Algorithm



Guessed y instead of y^* on example x with features $f(x)$

$$w_y = w'_y - \tau f(x)$$
$$w_{y^*} = w'_{y^*} + \tau f(x)$$

Minimum Correcting Update

$$w_y = w'_y - \tau f(x)$$
$$w_{y^*} = w'_{y^*} + \tau f(x)$$

$$w_{y^*} \cdot f \geq w_y \cdot f + 1$$

$$\Downarrow$$

$$(w'_{y^*} + \tau f) \cdot f = (w'_y - \tau f) \cdot f + 1$$

$$\tau = \frac{(w'_y - w'_{y^*}) \cdot f + 1}{2f \cdot f}$$

Maximum Step Size

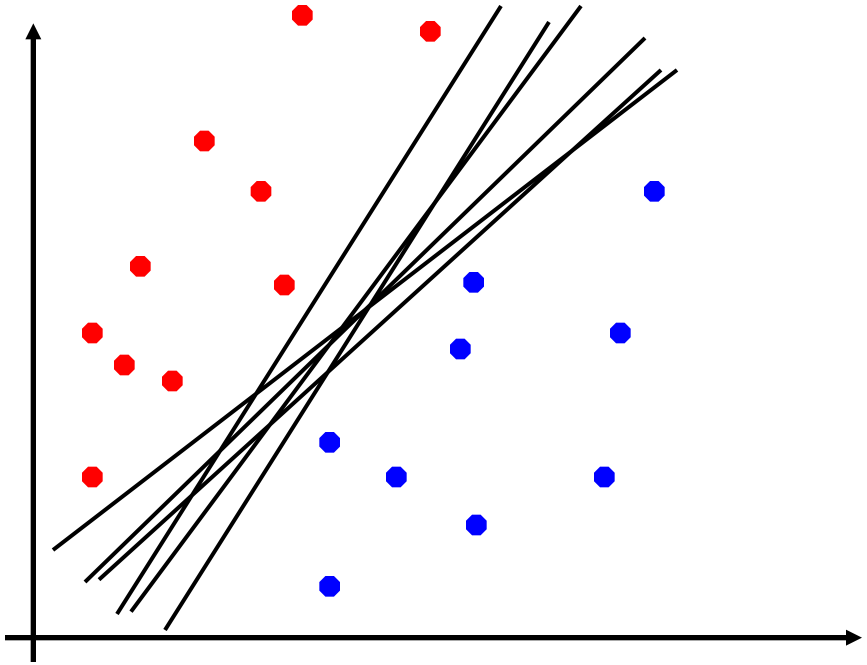
- In practice, it's also bad to make updates that are too large
  - Example may be labeled incorrectly
  - You may not have enough features
  - Solution: cap the maximum possible value of τ with some constant C

$$\tau^* = \min\left(\frac{(w'_y - w'_{y^*}) \cdot f + 1}{2f \cdot f}, C\right)$$

  - Corresponds to an optimization that assumes non-separable data
  - Usually converges faster than perceptron
  - Usually better, especially on noisy data

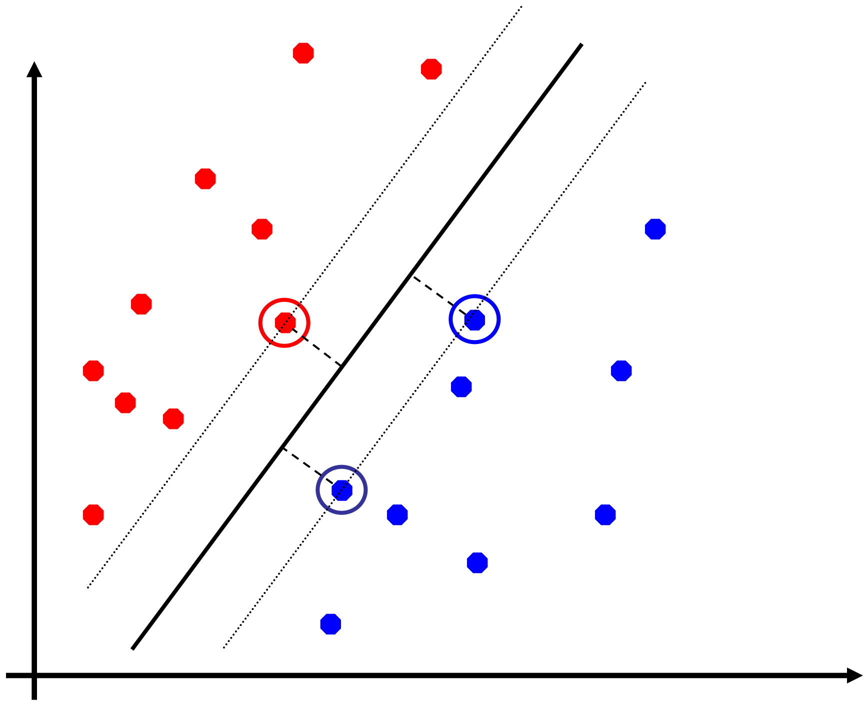
Linear Separators

- Which of these linear separators is optimal?



Support Vector Machines

- Maximizing the margin: good according to intuition, theory, practice
- Only support vectors matter; other training examples are ignorable
- Support vector machines (SVMs) find the separator with max margin
- Basically, SVMs are MIRA where you optimize over all examples at once



MIRA

$$w_{y^*} \cdot f(x_i) \geq w_y \cdot f(x_i) + 1$$

SVM

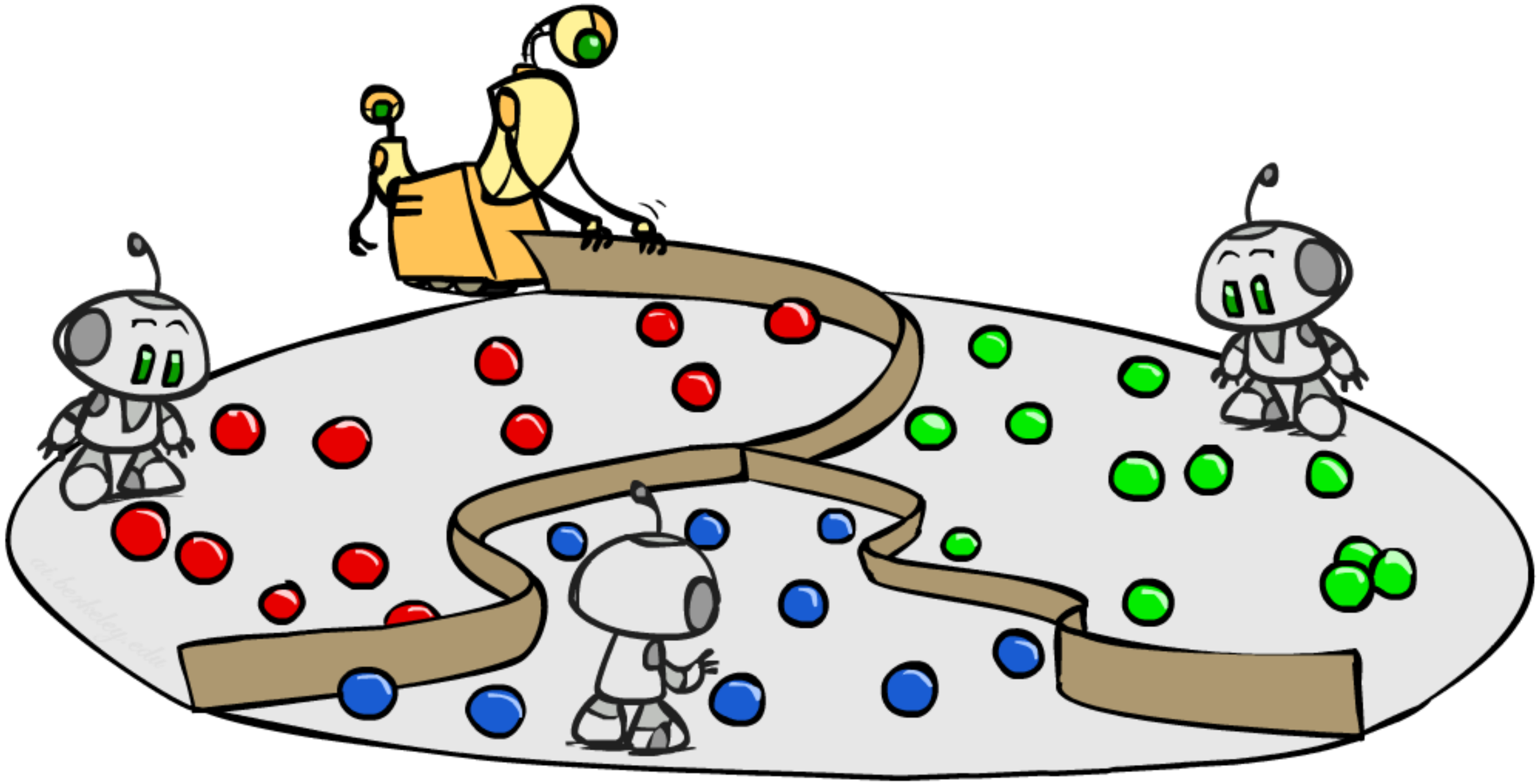
$$\forall i, y \; w_{y^*} \cdot f(x_i) \geq w_y \cdot f(x_i) + 1$$

Classification: Comparison

- Naïve Bayes
  - Builds a model training data
  - Gives prediction probabilities
  - Strong assumptions about feature independence
  - One pass through data (counting)

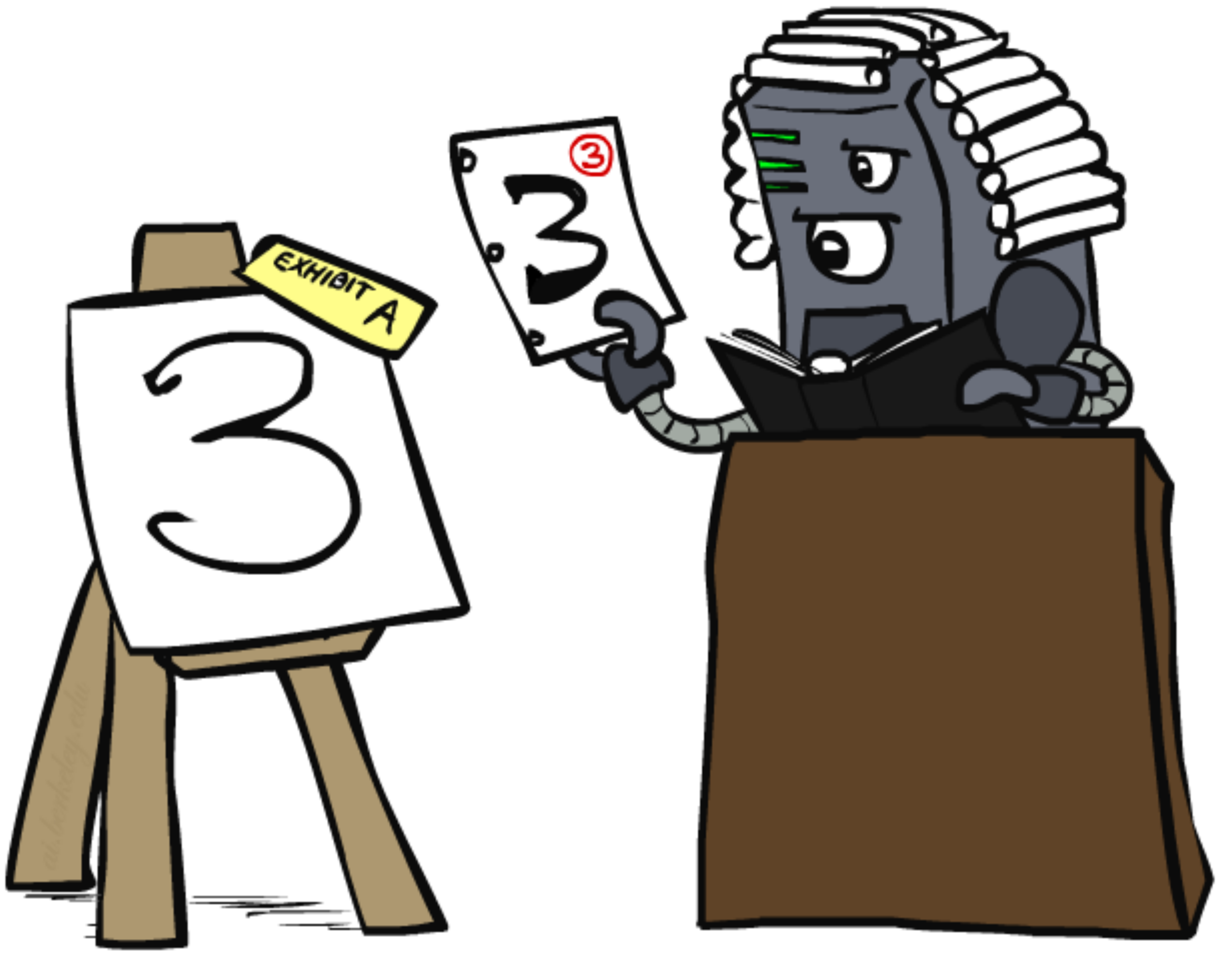
- Perceptrons / MIRA:
  - Makes less assumptions about data
  - Mistake-driven learning
  - Multiple passes through data (prediction)
  - Often more accurate

kNN and Kernelized Perceptrons

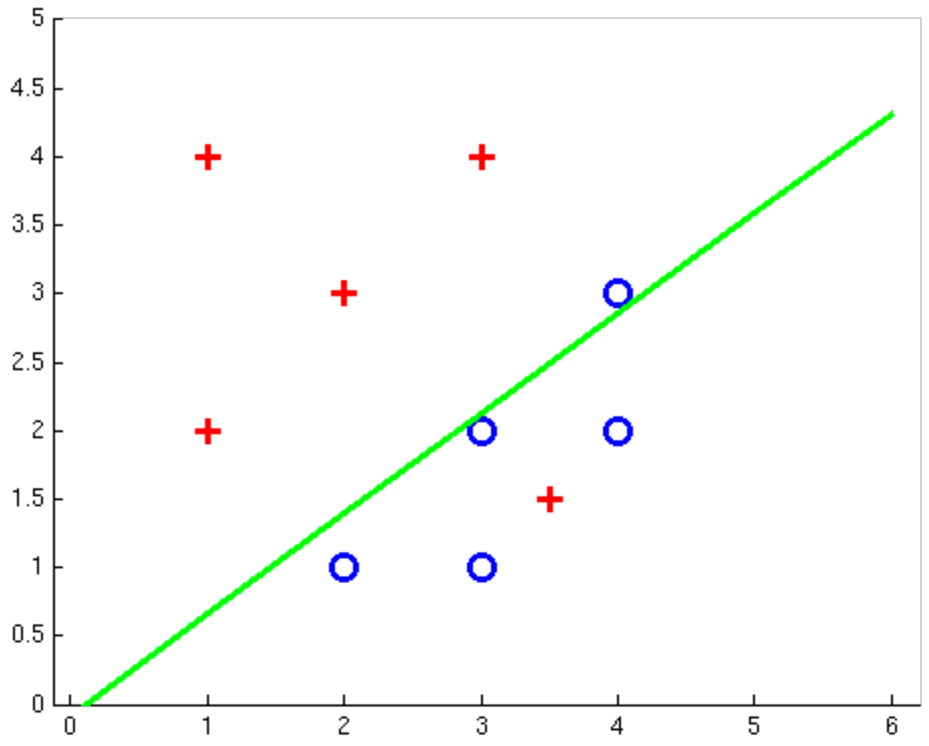


Slides Courtesy of Dan Klein and Pieter Abbeel --- University of California, Berkeley

Case-Based Learning

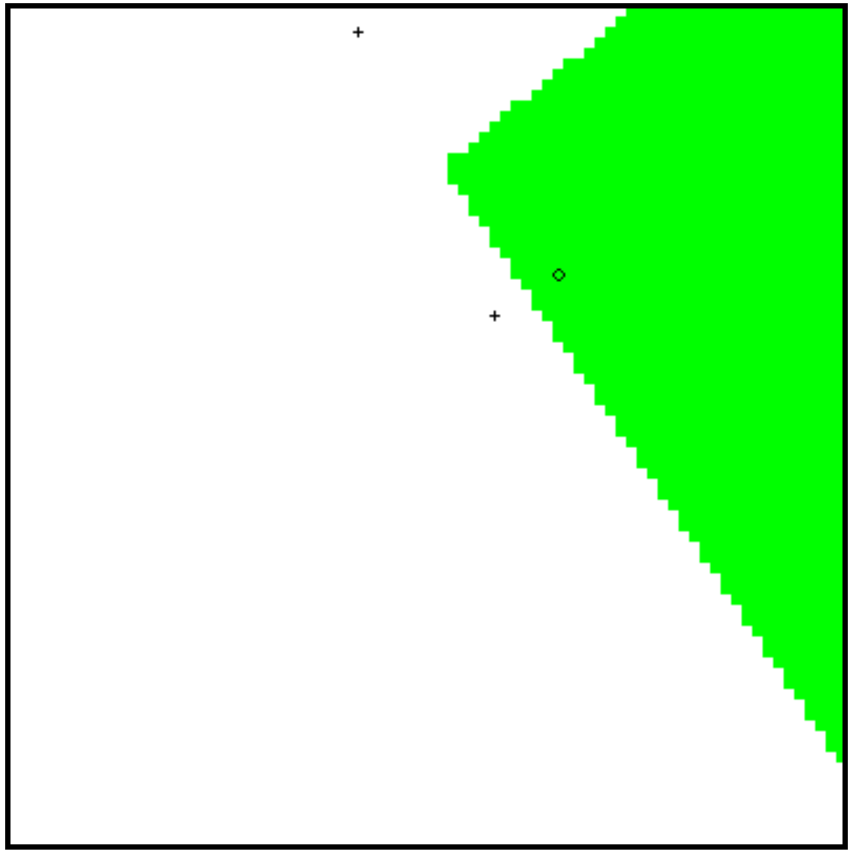


Non-Separable Data



Case-Based Reasoning

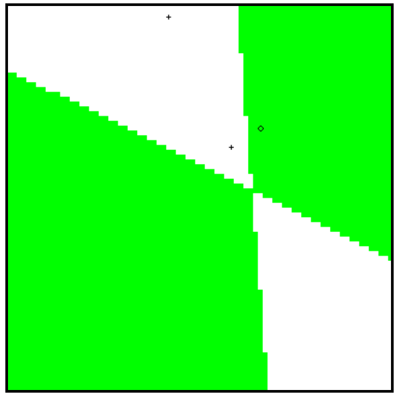
- Classification from similarity
  - Case-based reasoning
  - Predict an instance's label using similar instances
- Nearest-neighbor classification
  - 1-NN: copy the label of the most similar data point
  - K-NN: vote the k nearest neighbors (need a weighting scheme)
  - Key issue: how to define similarity
  - Trade-offs: Small k gives relevant neighbors, Large k gives smoother functions



http://www.cs.cmu.edu/~zhuxj/courseproject/knndemo/KNN.html

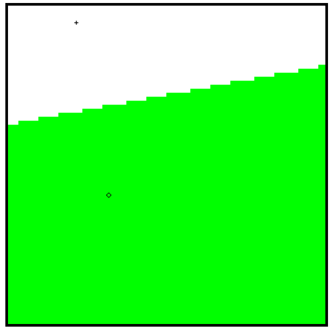
Parametric / Non-Parametric

- Parametric models:
  - Fixed set of parameters
  - More data means better settings
- Non-parametric models:
  - Complexity of the classifier increases with data
  - Better in the limit, often worse in the non-limit
- (K)NN is non-parametric

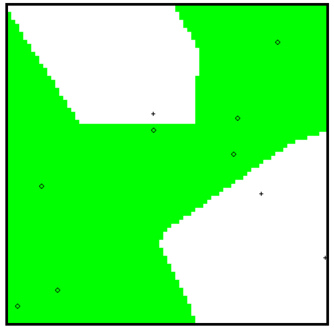


Truth

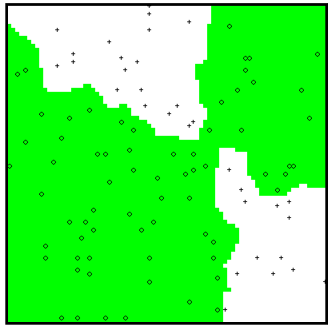
2 Examples



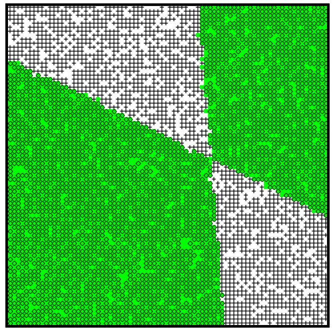
10 Examples



100 Examples



10000 Examples



Nearest-Neighbor Classification

- Nearest neighbor for digits:
  - Take new image
  - Compare to all training images
  - Assign based on closest example

0

1

2

0

1

2

- Encoding: image is vector of intensities:

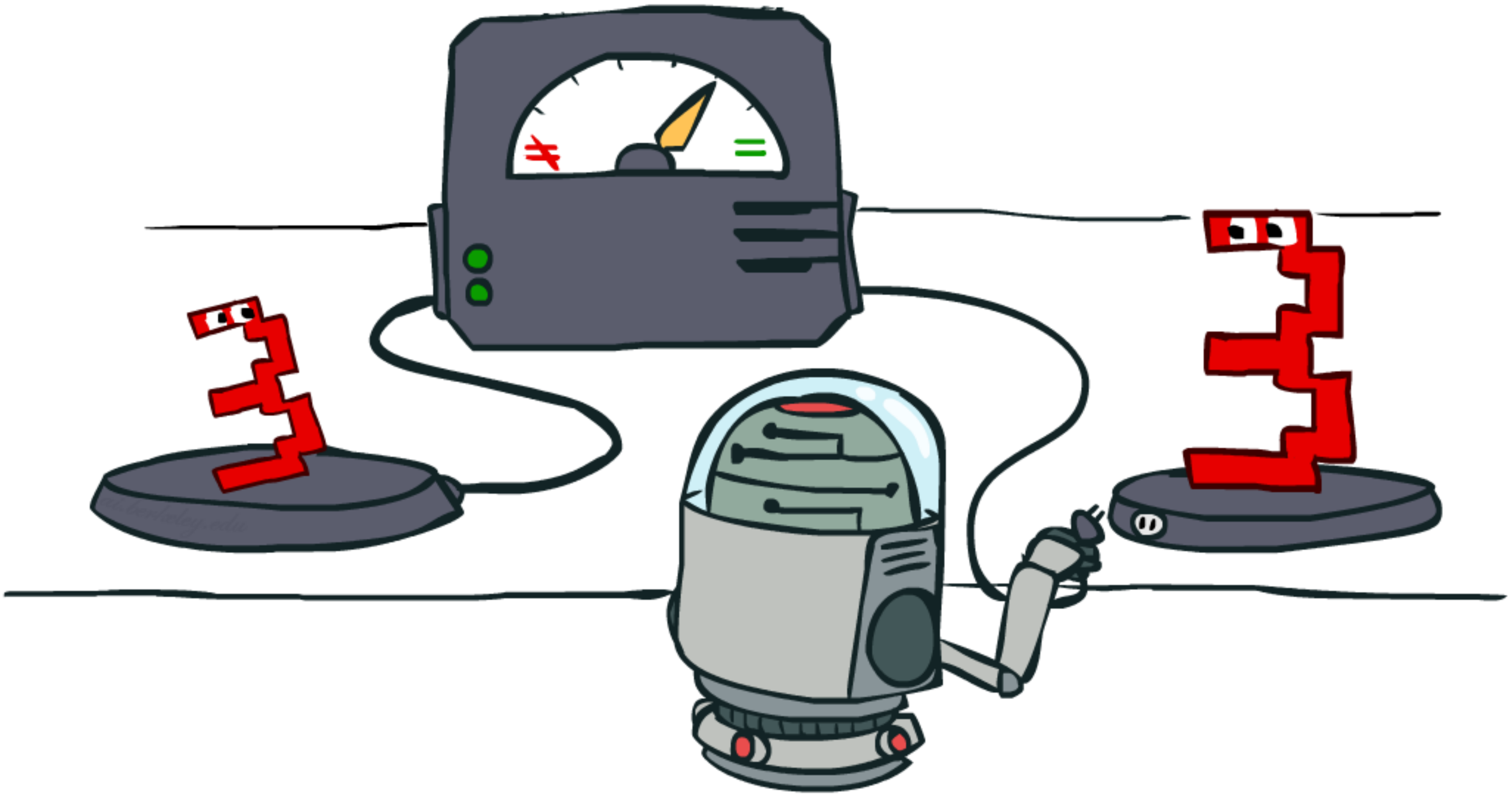
 $= \langle 0.0 \;\; 0.0 \;\; 0.3 \;\; 0.8 \;\; 0.7 \;\; 0.1 \ldots 0.0 \rangle$

- What's the similarity function?
  - Dot product of two images vectors?

$$\text{sim}(x, x') = x \cdot x' = \sum_i x_i x'_i$$

  - Usually normalize vectors so ||x|| = 1
  - min = 0 (when?), max = 1 (when?)

Similarity Functions



Basic Similarity

- Many similarities based on feature dot products:

$$\text{sim}(x, x') = f(x) \cdot f(x') = \sum_i f_i(x) f_i(x')$$

- If features are just the pixels:

$$\text{sim}(x, x') = x \cdot x' = \sum_i x_i x'_i$$

- Note: not all similarities are of this form

Invariant Metrics

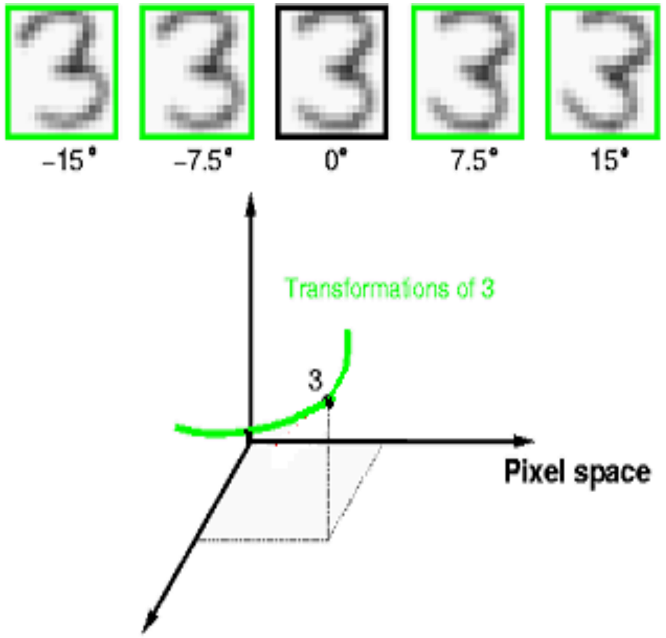
- Better similarity functions use knowledge about vision
- Example: invariant metrics:
  - Similarities are invariant under certain transformations
  - Rotation, scaling, translation, stroke-thickness…
  - E.g:

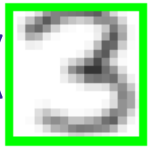
    - 16 x 16 = 256 pixels; a point in 256-dim space
    - These points have small similarity in R^{256} (why?)
  - How can we incorporate such invariances into our similarities?

This and next few slides adapted from Xiao Hu, UIUC

Rotation Invariant Metrics

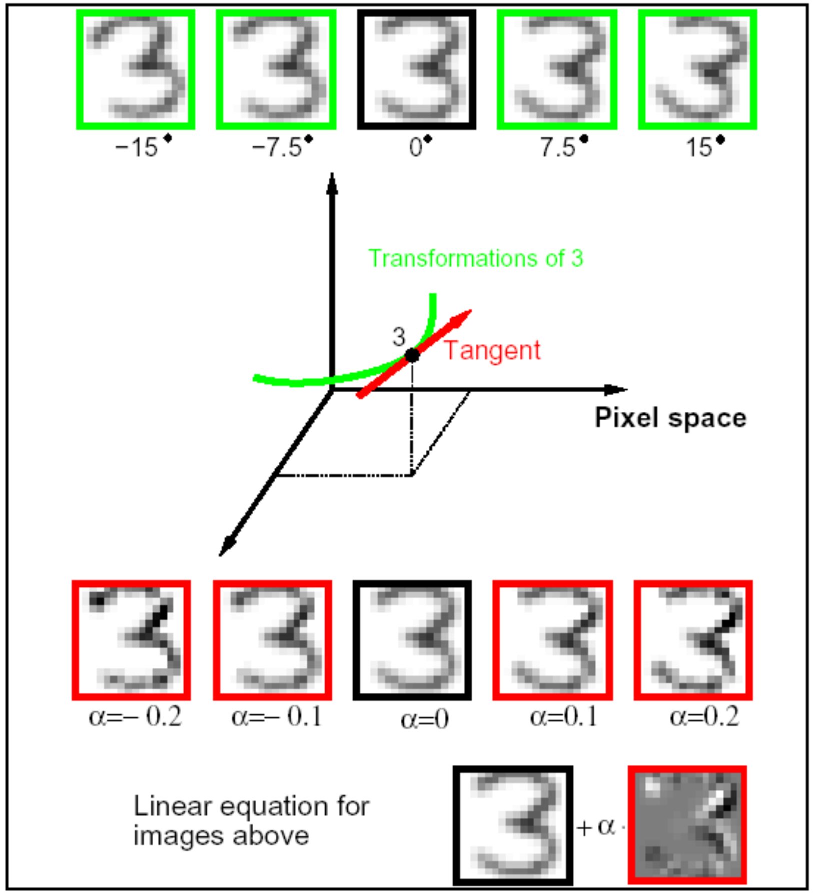


- Each example is now a curve in R^{256}
- Rotation invariant similarity:

s'=max s(r(), r())

- E.g. highest similarity between images' rotation lines

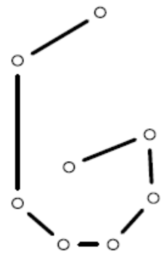
Tangent Families



- Problems with s':
  - Hard to compute
  - Allows large transformations (e.g. 6 $\rightarrow$ 9)
- Tangent distance:
  - 1st order approximation at original points.
    - Easy to compute
    - Models small rotations

Template Deformation

- Deformable templates:
  - An “ideal” version of each category
  - Best-fit to image using min variance
  - Cost for high distortion of template
  - Cost for image points being far from distorted template
- Used in many commercial digit recognizers



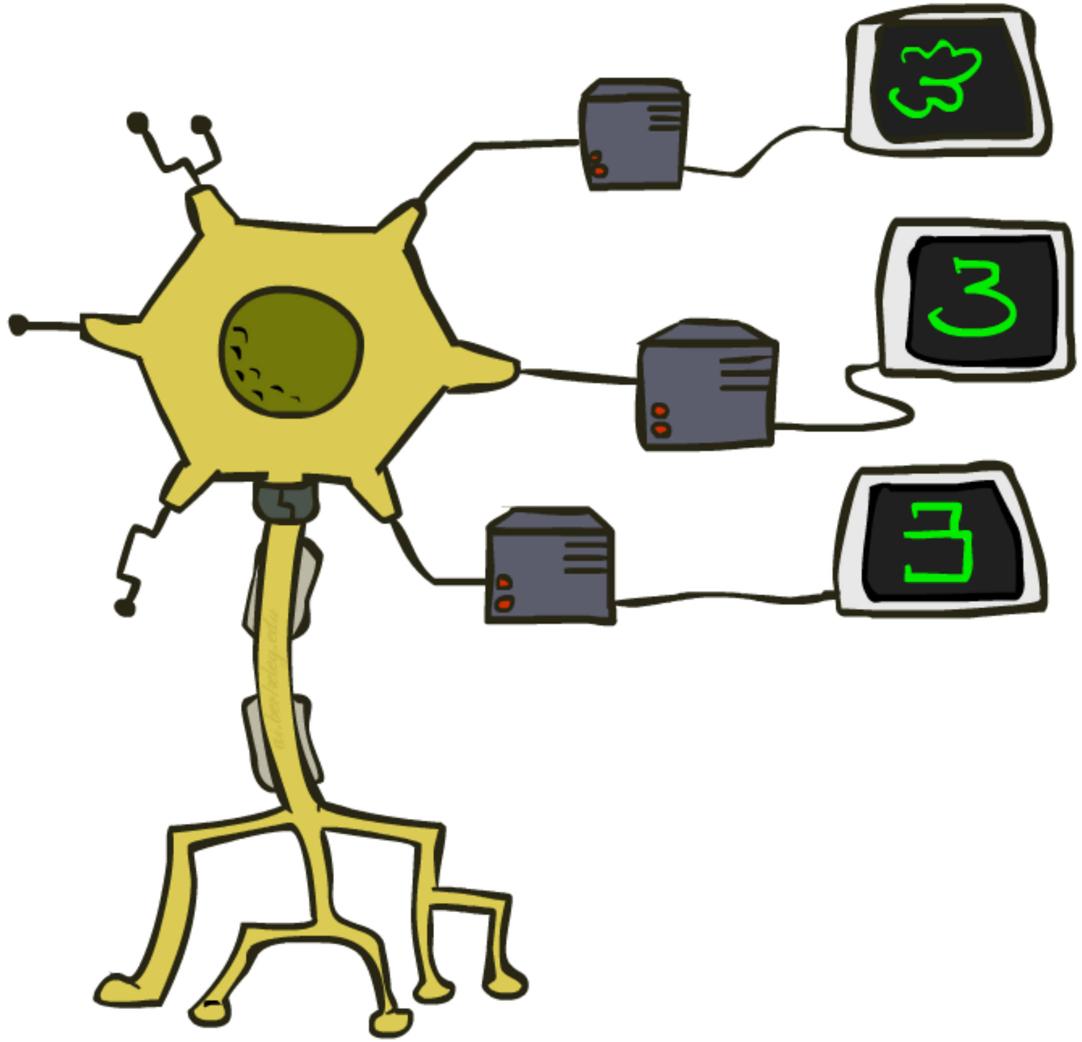
Examples from [Hastie 94]

A Tale of Two Approaches…

- Nearest neighbor-like approaches
  - Can use fancy similarity functions
  - Don’t actually get to do explicit learning

- Perceptron-like approaches
  - Explicit training to reduce empirical error
  - Can’t use fancy similarity, only linear
  - Or can they? Let’s find out!

Kernelization



Perceptron Weights

- What is the final value of a weight w_y of a perceptron?
  - Can it be any real vector?
  - No! It's built by adding up inputs.

$$w_y = \mathbf{0} + f(x_1) - f(x_5) + \ldots$$

$$w_y = \sum_i \alpha_{i,y} f(x_i)$$

- Can reconstruct weight vectors (the primal representation) from update counts (the dual representation)

$$\alpha_y = \langle \alpha_{1,y} \;\; \alpha_{2,y} \;\; \ldots \;\; \alpha_{n,y} \rangle$$

Dual Perceptron

- How to classify a new example x?

$$\text{score}(y, x) = w_y \cdot f(x)$$

$$= \left(\sum_i \alpha_{i,y} \, f(x_i) \right) \cdot f(x)$$

$$= \sum_i \alpha_{i,y} \left(f(x_i) \cdot f(x) \right)$$

$$= \sum_i \alpha_{i,y} \; K(x_i, x)$$

- If someone tells us the value of K for each pair of examples, never need to build the weight vectors (or the feature vectors)!

Training the Dual Perceptron

- Start with zero counts (alpha)
- Pick up training instances one by one
- Try to classify x_n,

$$y = \arg\max_y \sum_i \alpha_{i,y} K(x_i, x_n)$$

- If correct, no change!
- If wrong: lower count of wrong class (for this instance), raise count of right class (for this instance)

$$\alpha_{y,n} = \alpha_{y,n} - 1 \qquad w_y = w_y - f(x_n)$$

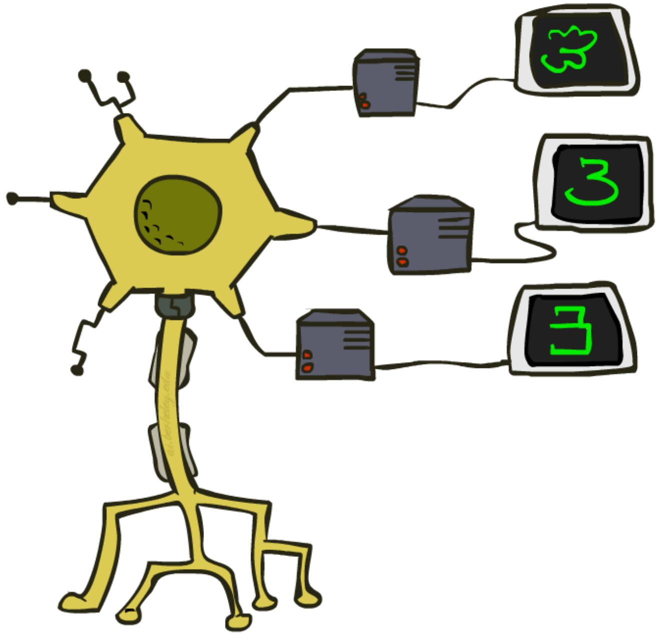
$$\alpha_{y^*,n} = \alpha_{y^*,n} + 1 \qquad w_{y^*} = w_{y^*} + f(x_n)$$

Kernelized Perceptron

- If we had a black box (kernel) K that told us the dot product of two examples x and x':
  - Could work entirely with the dual representation
  - No need to ever take dot products ("kernel trick")

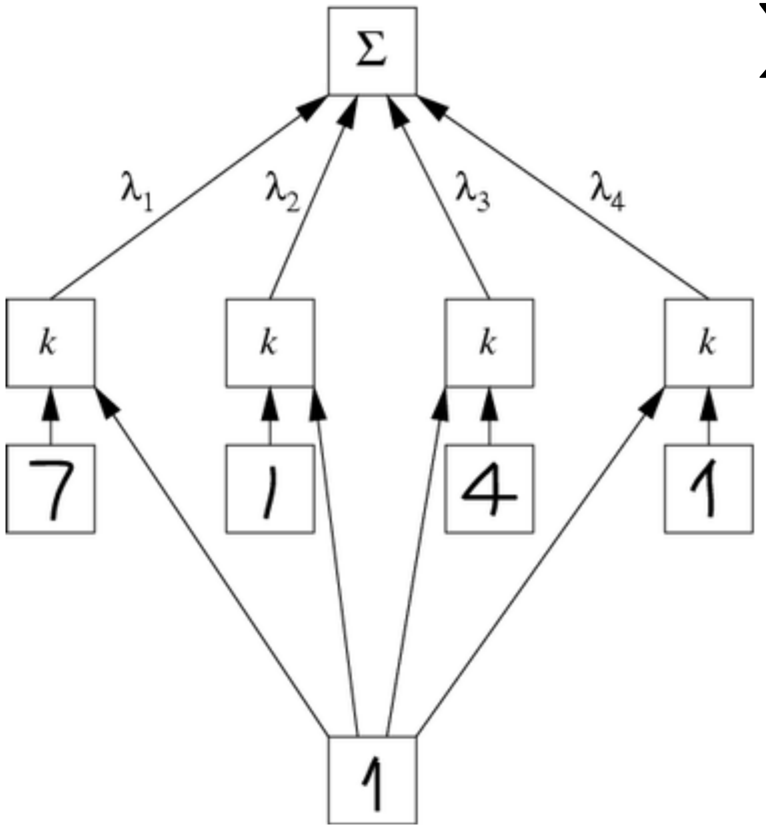
$$\text{score}(y, x) = w_y \cdot f(x)$$

$$= \sum_i \alpha_{i,y} \, K(x_i, x)$$



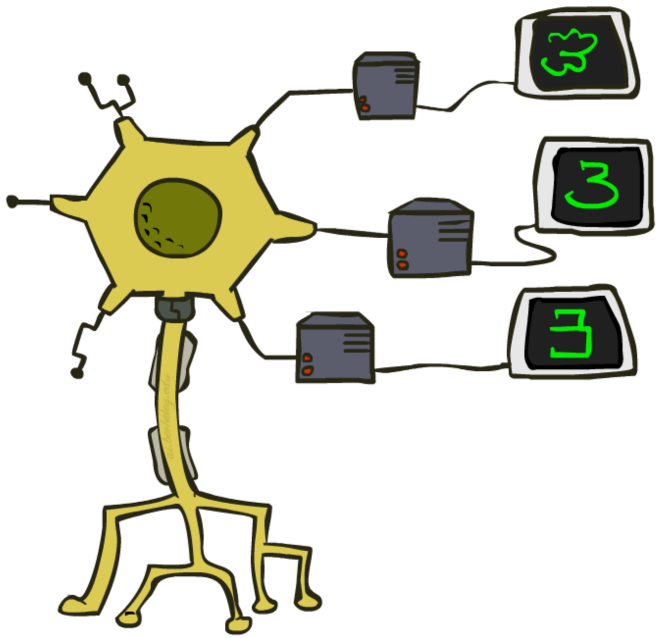
- Like nearest neighbor – work with black-box similarities
- Downside: slow if many examples get nonzero alpha

Kernelized Perceptron Structure



$$\sum = \text{score}(c, x)$$

$$\lambda_i = \alpha_{c,i}$$



Kernels: Who Cares?

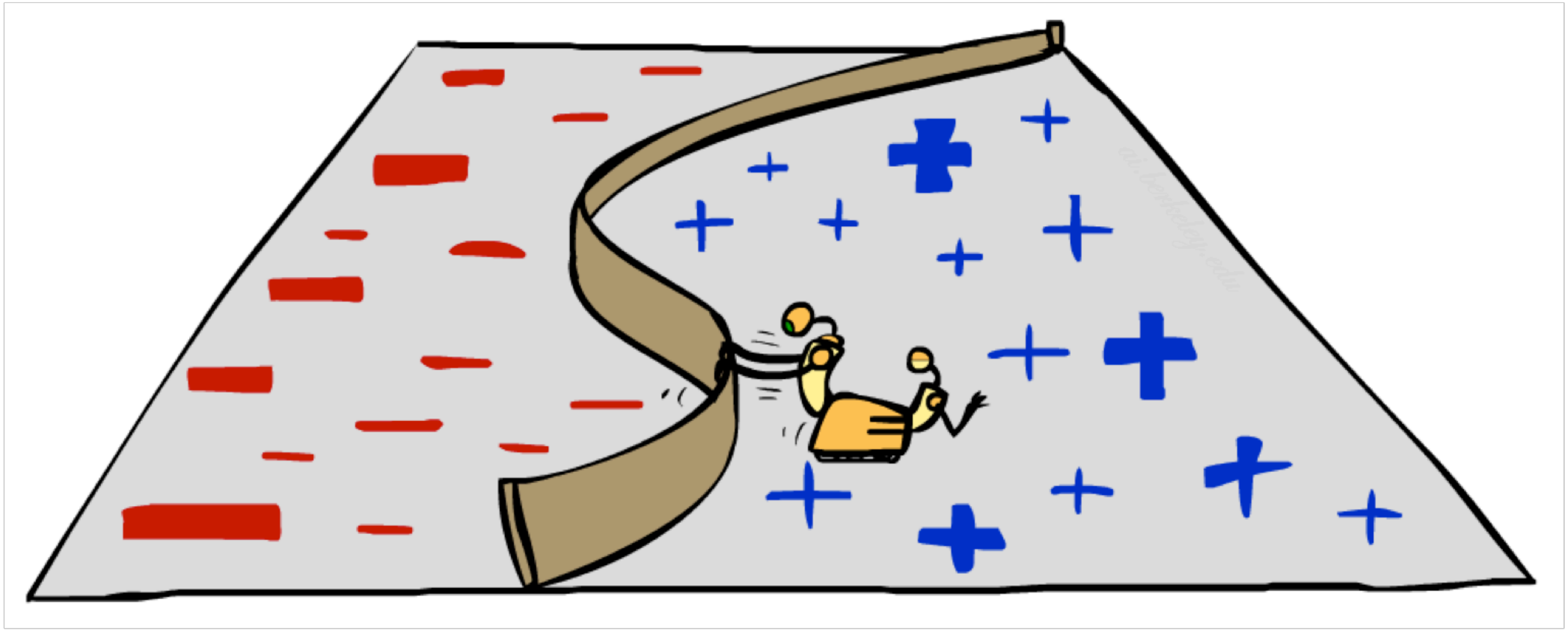
- So far: a very strange way of doing a very simple calculation

- “Kernel trick”: we can substitute any* similarity function in place of the dot product

- Lets us learn new kinds of hypotheses

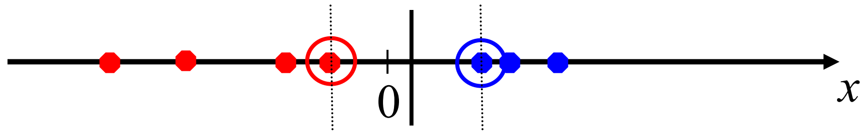
* Fine print: if your kernel doesn’t satisfy certain technical requirements, lots of proofs break. E.g. convergence, mistake bounds. In practice, illegal kernels *sometimes* work (but not always).

Non-Linearity

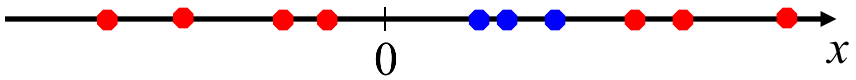


Non-Linear Separators

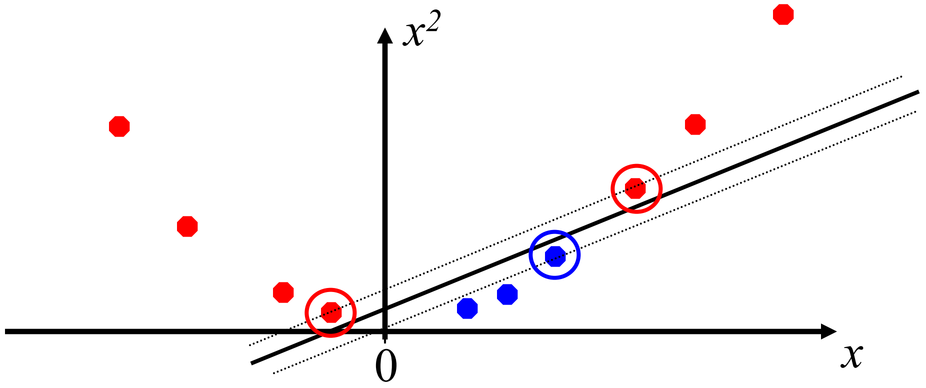
- Data that is linearly separable works out great for linear decision rules:



- But what are we going to do if the dataset is just too hard?



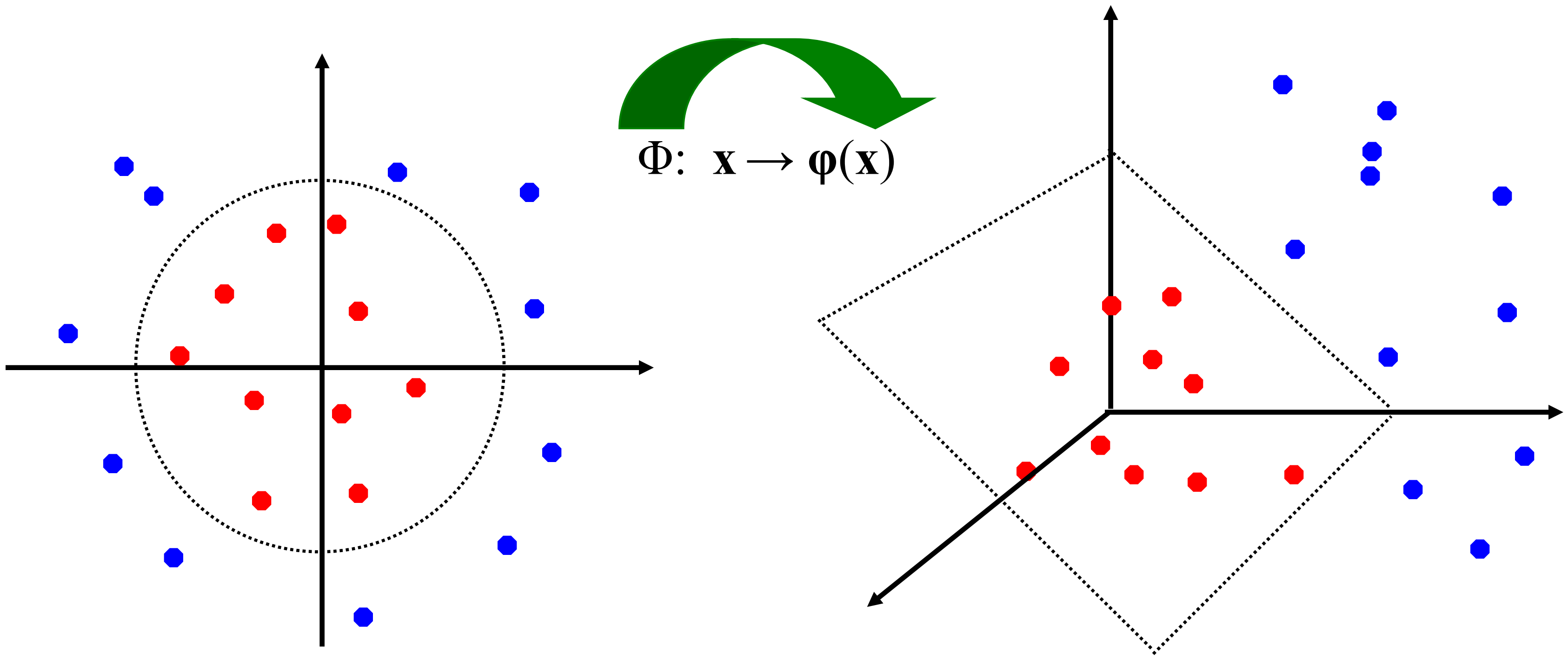
- How about… mapping data to a higher-dimensional space:



This and next few slides adapted from Ray Mooney, UT

Non-Linear Separators

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Some Kernels

- Kernels implicitly map original vectors to higher dimensional spaces, take the dot product there, and hand the result back

- Linear kernel: $$K(x, x') = x' \cdot x' = \sum_i x_i x'_i$$

- Quadratic kernel: $$K(x, x') = (x \cdot x' + 1)^2$$
$$= \sum_{i,j} x_i x_j \, x'_i x'_j + 2 \sum_i x_i \, x'_i + 1$$

- RBF: infinite dimensional representation
$$K(x, x') = \exp(-||x - x'||^2)$$

- Discrete kernels: e.g. string kernels

Why Kernels?

- Can't you just add these features on your own (e.g. add all pairs of features instead of using the quadratic kernel)?
  - Yes, in principle, just compute them
  - No need to modify any algorithms
  - But, number of features can get large (or infinite)
  - Some kernels not as usefully thought of in their expanded representation, e.g. RBF kernels

- Kernels let us compute with these features implicitly
  - Example: implicit dot product in quadratic kernel takes much less space and time per dot product
  - Of course, there's the cost for using the pure dual algorithms: you need to compute the similarity to every training item

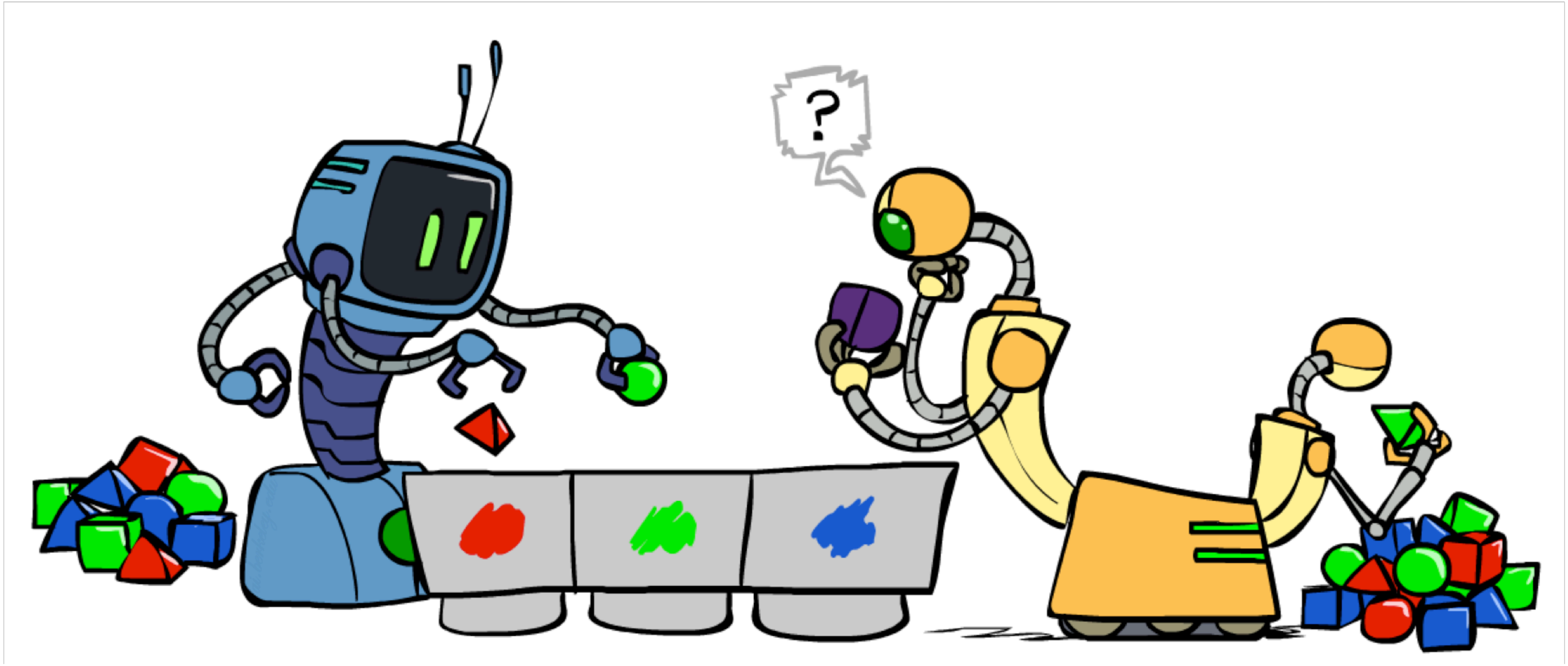
Recap: Classification

- Classification systems:
  - Supervised learning
  - Make a prediction given evidence
  - We've seen several methods for this
  - Useful when you have labeled data

Clustering

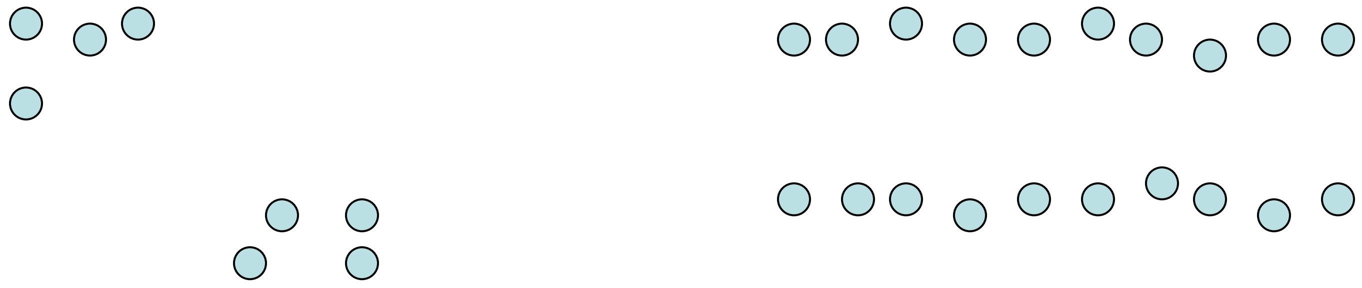
- Clustering systems:
  - Unsupervised learning
  - Detect patterns in unlabeled data
    - E.g. group emails or search results
    - E.g. find categories of customers
    - E.g. detect anomalous program executions
  - Useful when don't know what you're looking for
  - Requires data, but no labels
  - Often get gibberish

Clustering



Clustering

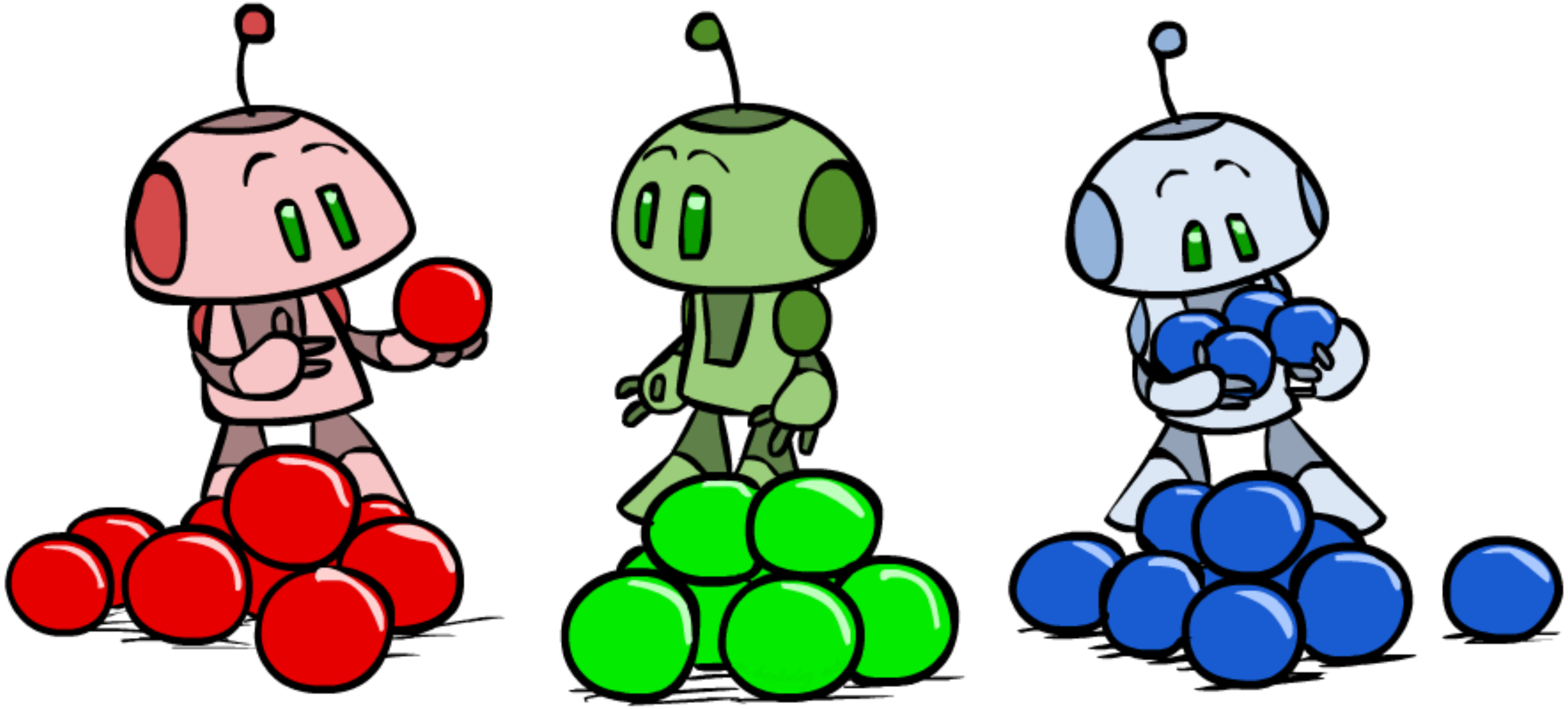
- Basic idea: group together similar instances
- Example: 2D point patterns



- What could “similar” mean?
  - One option: small (squared) Euclidean distance

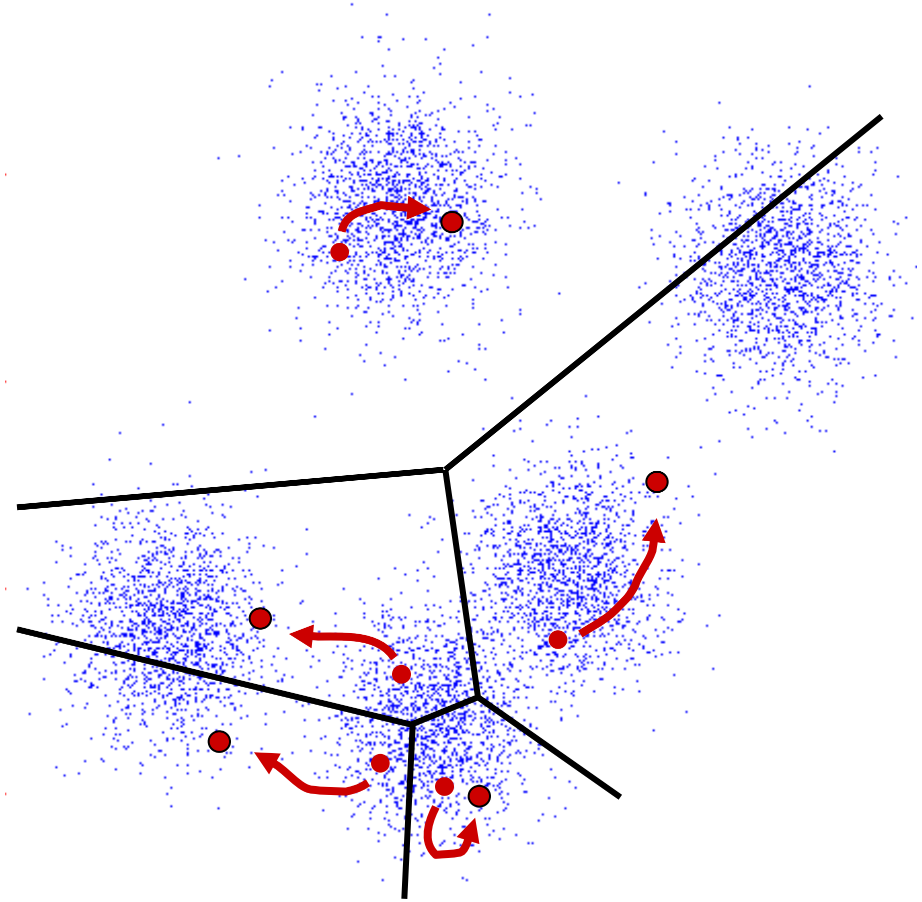
$$\text{dist}(x, y) = (x - y)^\top (x - y) = \sum_i (x_i - y_i)^2$$

K-Means

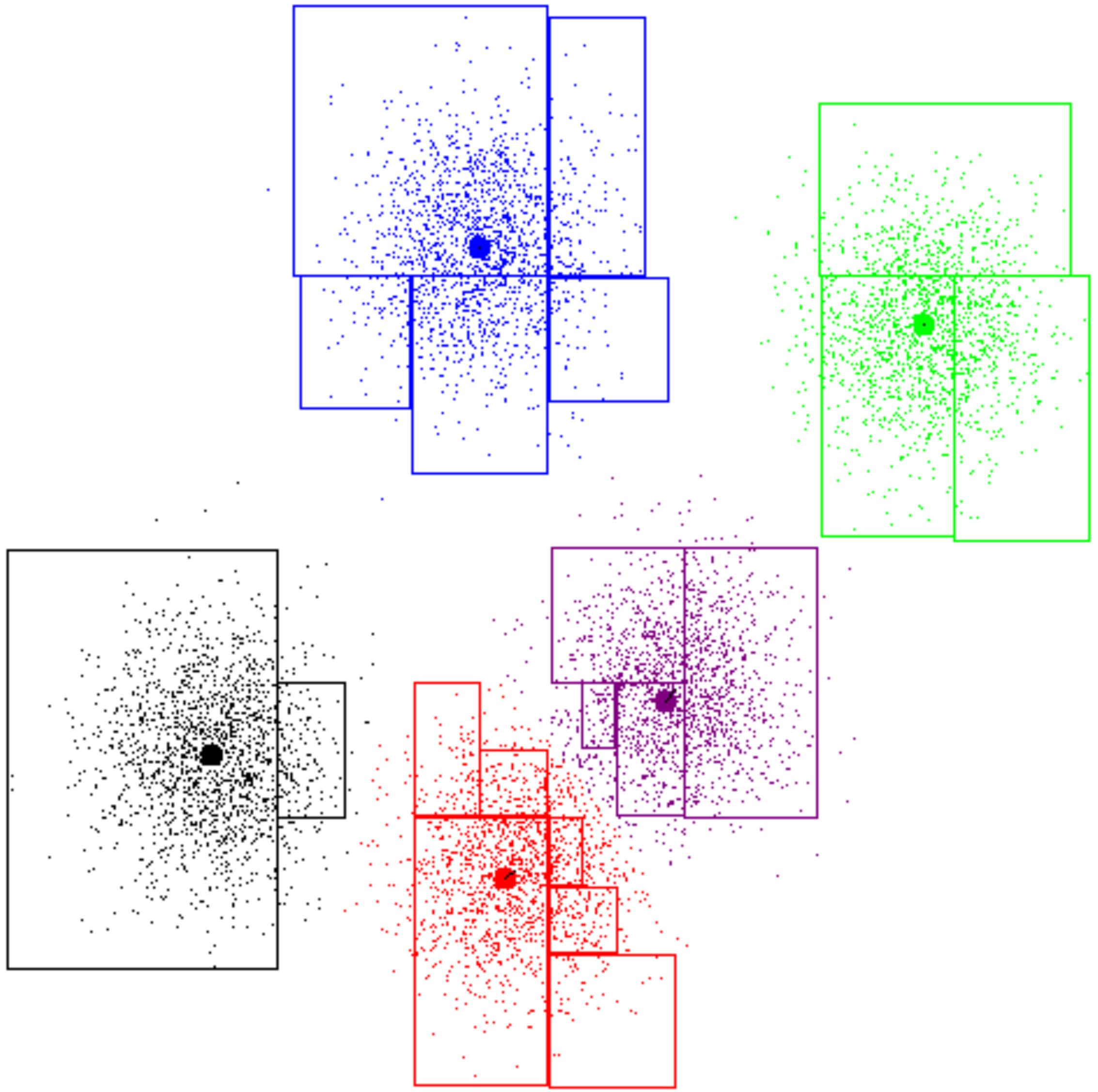


K-Means

- An iterative clustering algorithm
  - Pick K random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest mean
    - Assign each mean to the average of its assigned points
  - Stop when no points' assignments change



K-Means Example



K-Means as Optimization

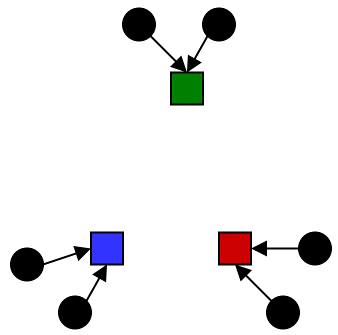
- Consider the total distance to the means:

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

points

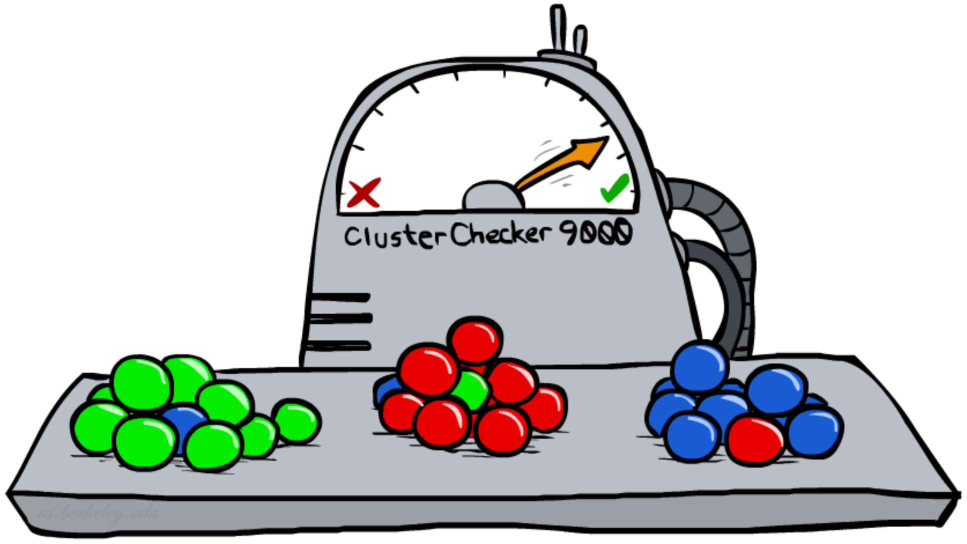
assignments

means



- Each iteration reduces phi

- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c



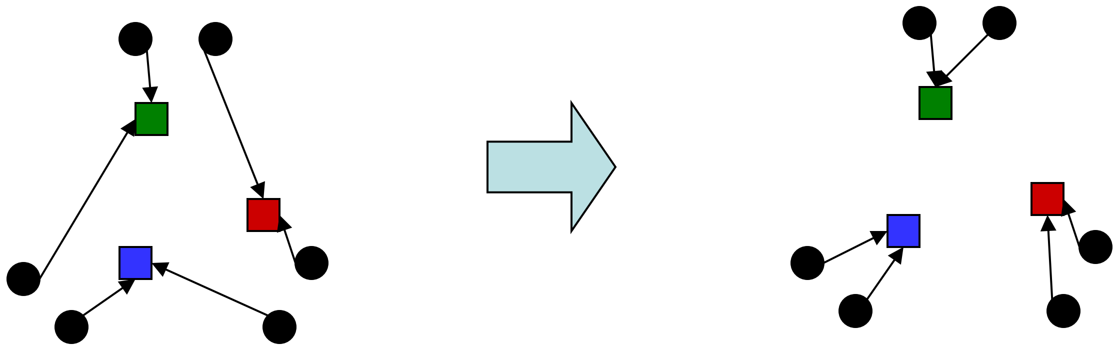
Phase I: Update Assignments

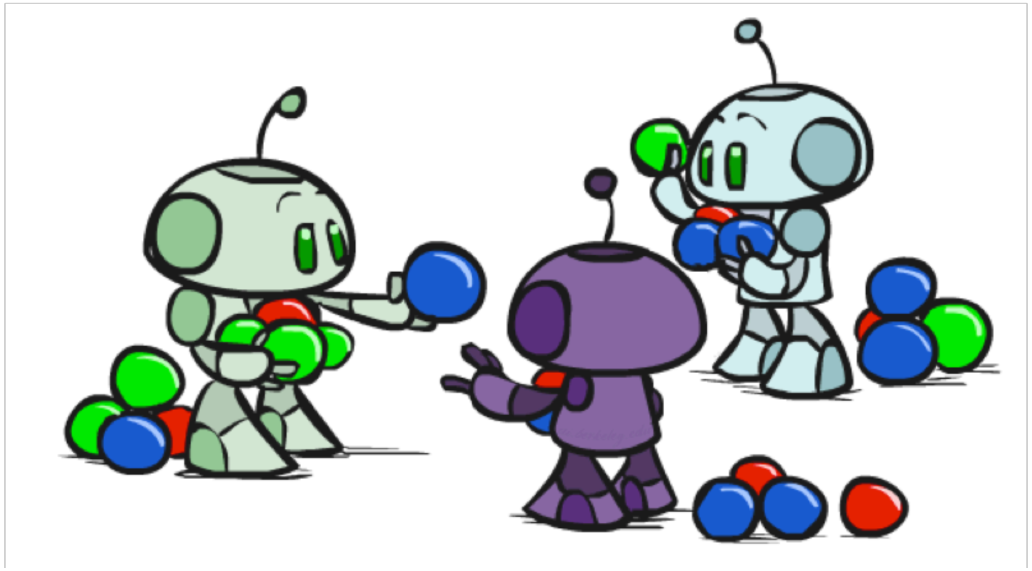
- For each point, re-assign to closest mean:

$$a_i = \underset{k}{\text{argmin}}\ \text{dist}(x_i, c_k)$$

- Can only decrease total distance phi!

$$\phi(\{x_i\},\{a_i\},\{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

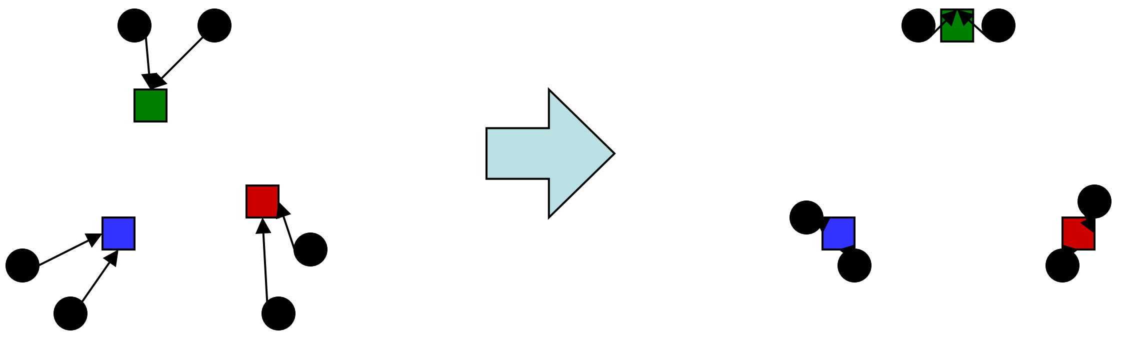




Phase II: Update Means

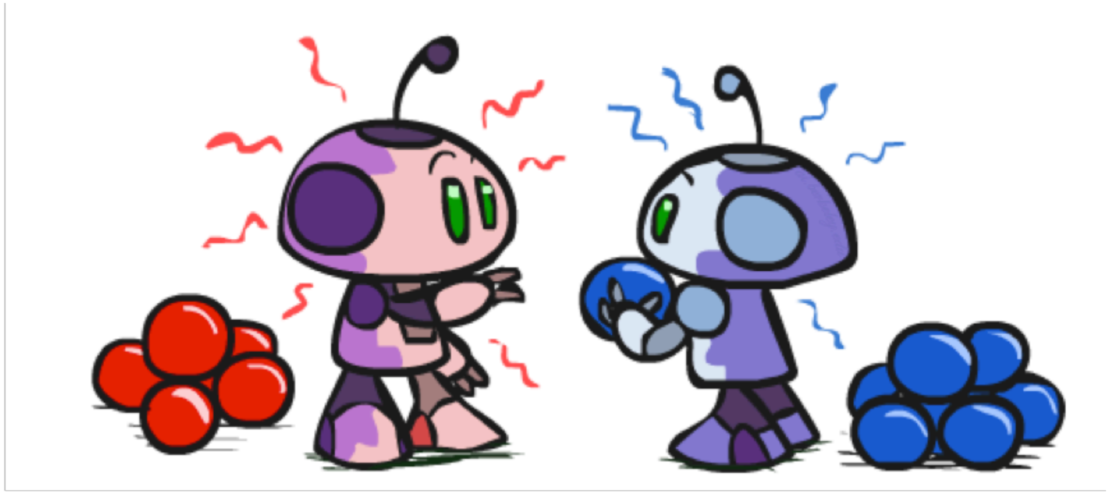
- Move each mean to the average of its assigned points:

$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$



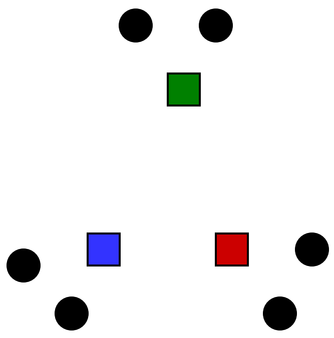
- Also can only decrease total distance… (Why?)

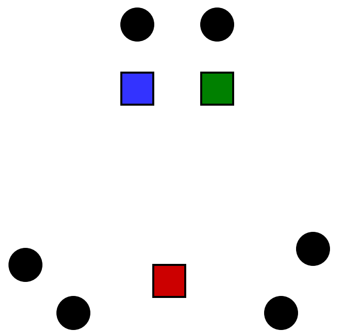
- Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean



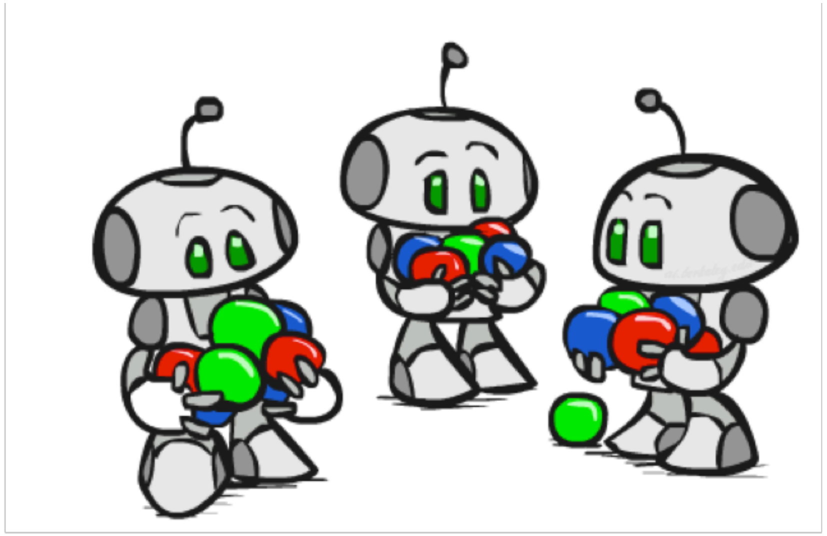
Initialization

- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?



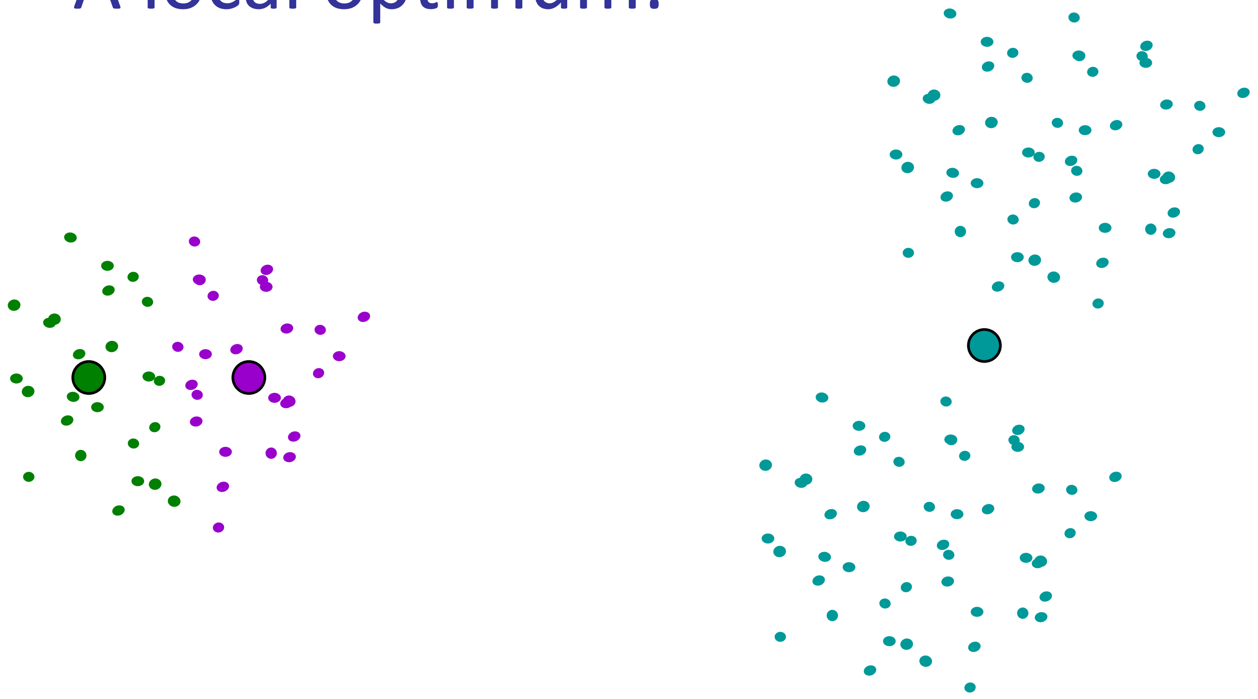


  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics

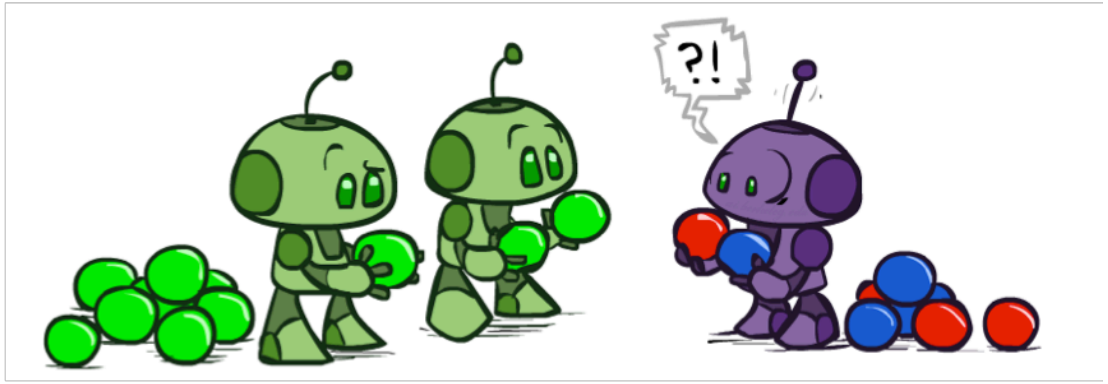


K-Means Getting Stuck

- A local optimum:

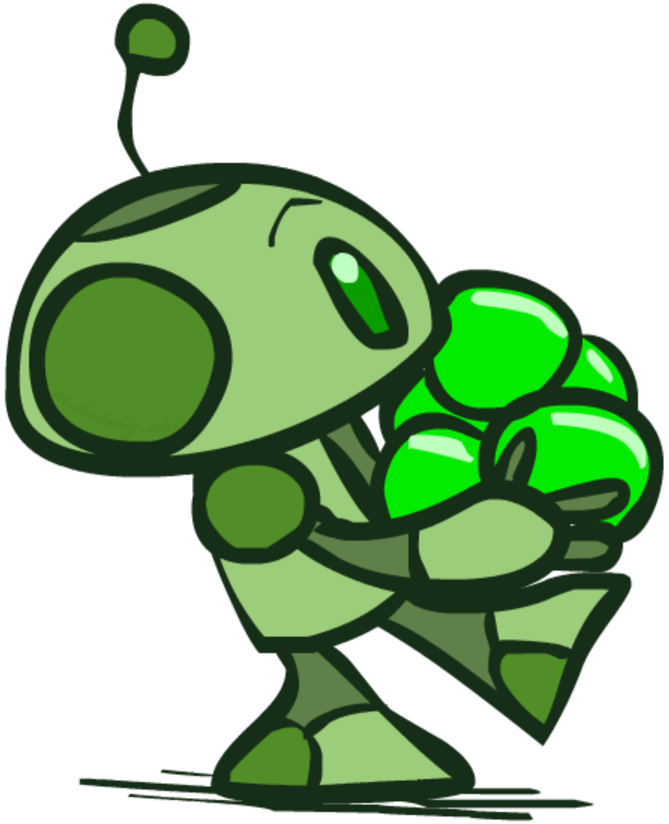


Why doesn't this work out like the earlier example, with the purple taking over half the blue?

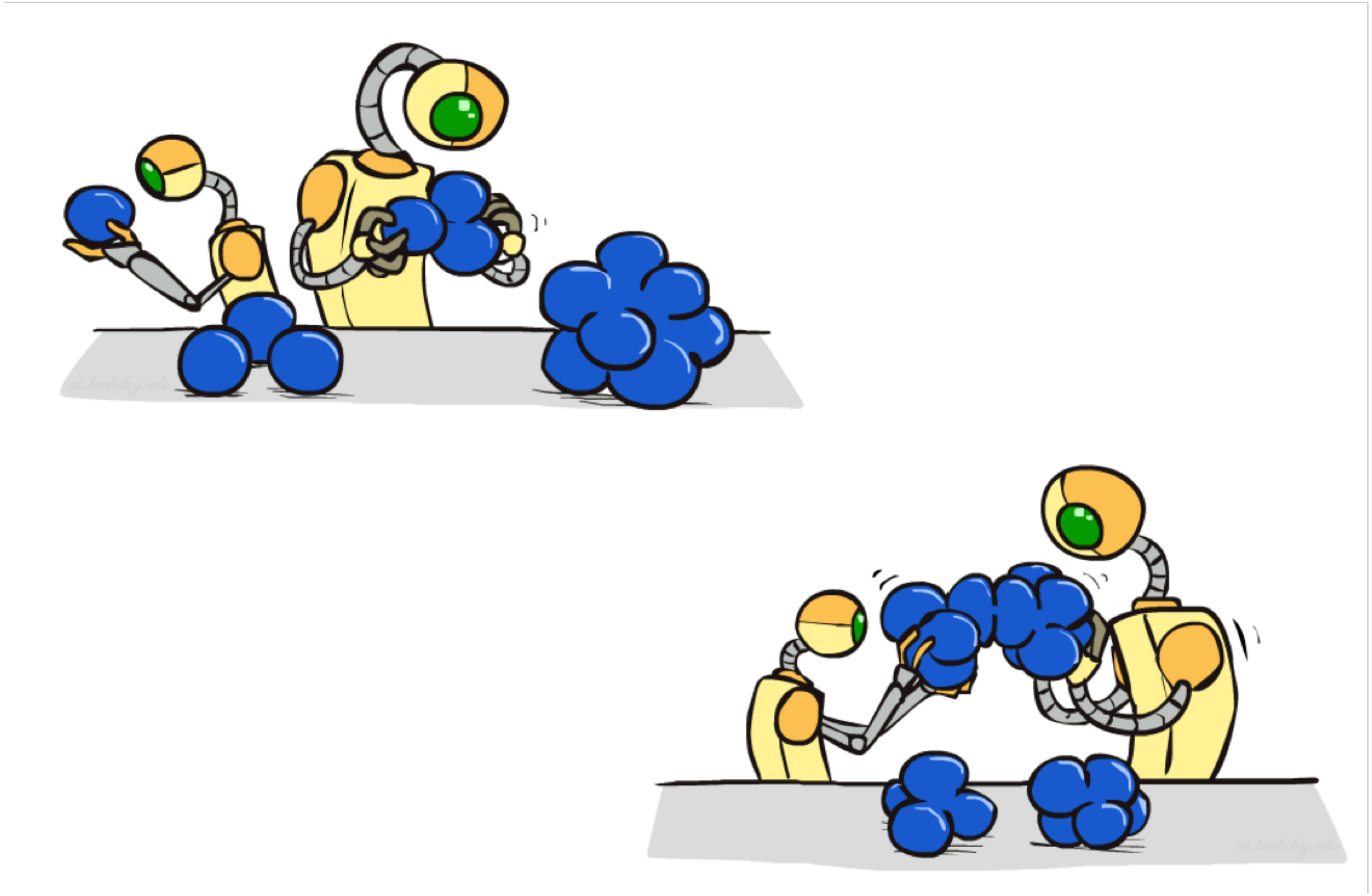


K-Means Questions

- Will K-means converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
  - If the patterns are very very clear?
- Will it find something interesting?
- Do people ever use it?
- How many clusters to pick?

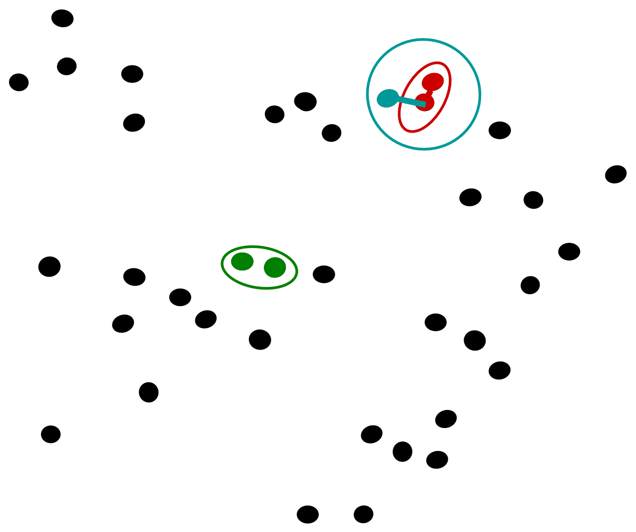


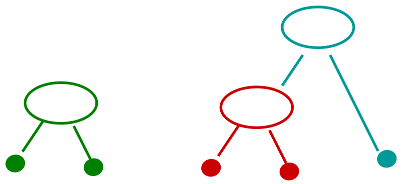
Agglomerative Clustering



Agglomerative Clustering

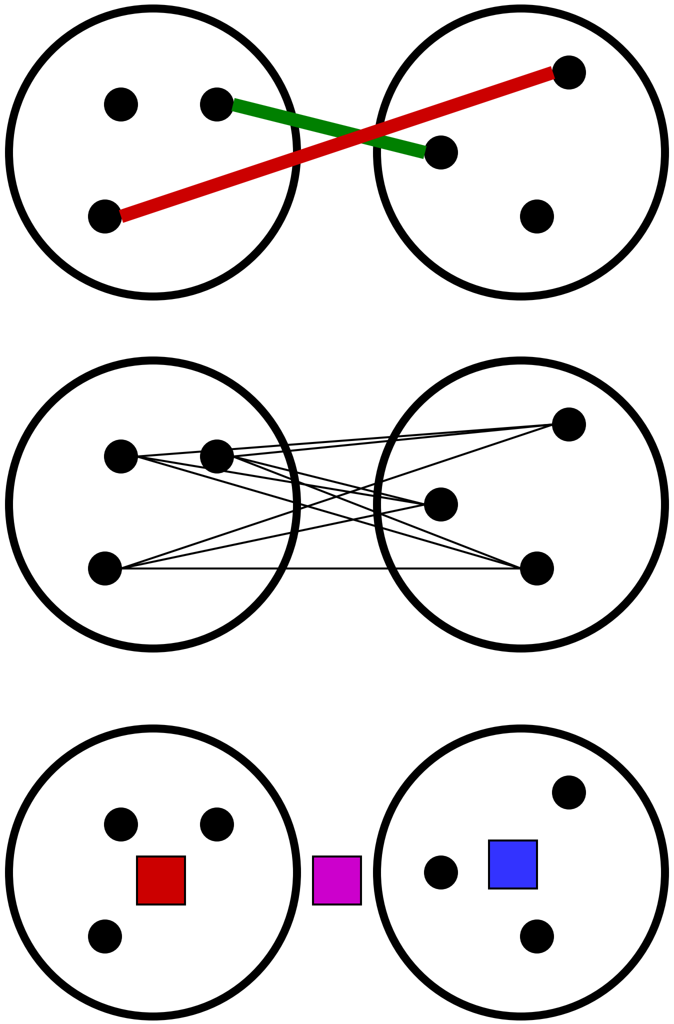
- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left
- Produces not one clustering, but a family of clusterings represented by a dendrogram



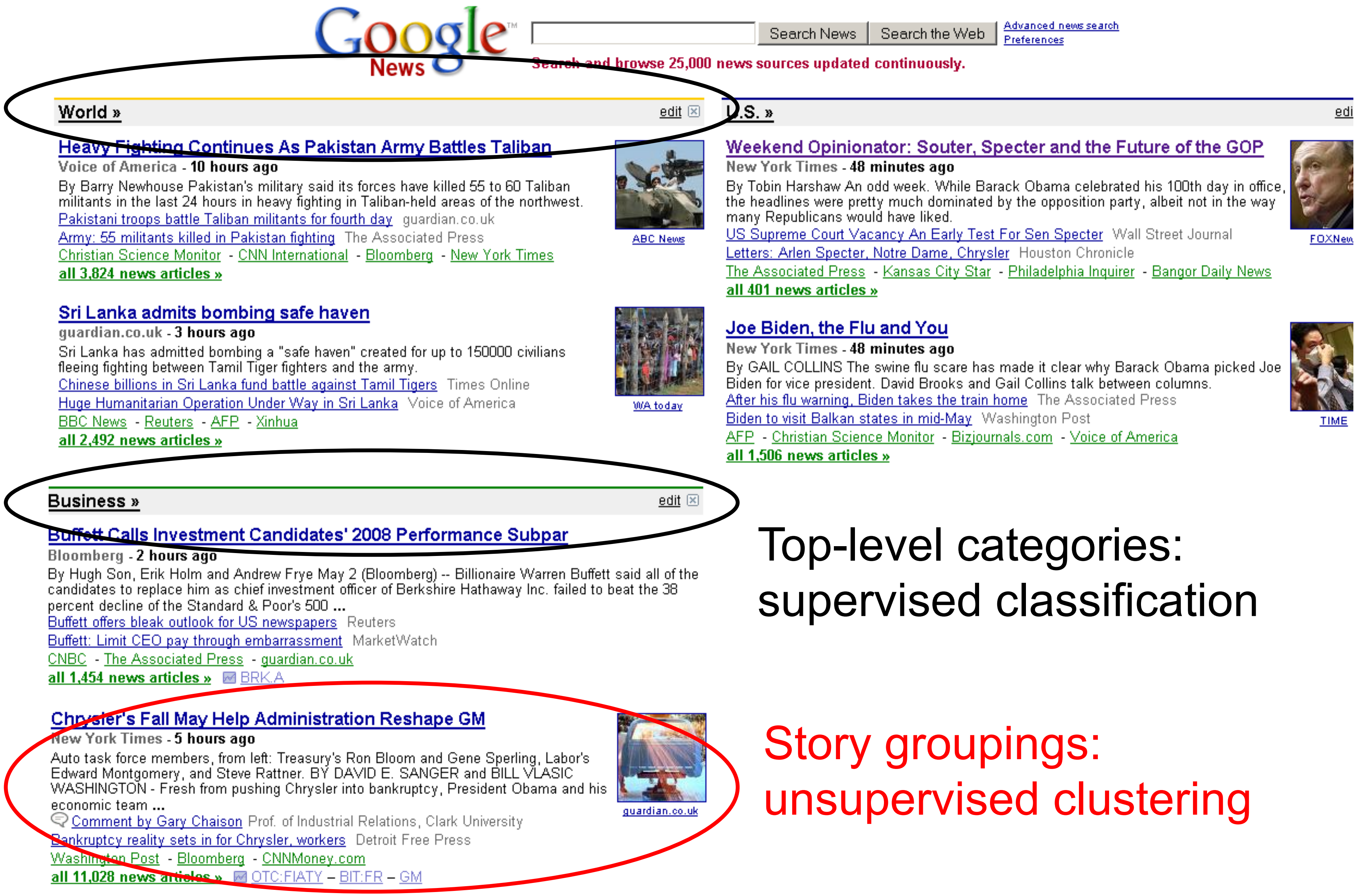


Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?
- Many options
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs
  - Ward's method (min variance, like k-means)
- Different choices create different clustering behaviors



Example: Google News



Top-level categories: supervised classification

Story groupings: unsupervised clustering

Example: K-Means

- [web demo]
  - http://www.cs.washington.edu/research/imagedatabase/demo/kmcluster/