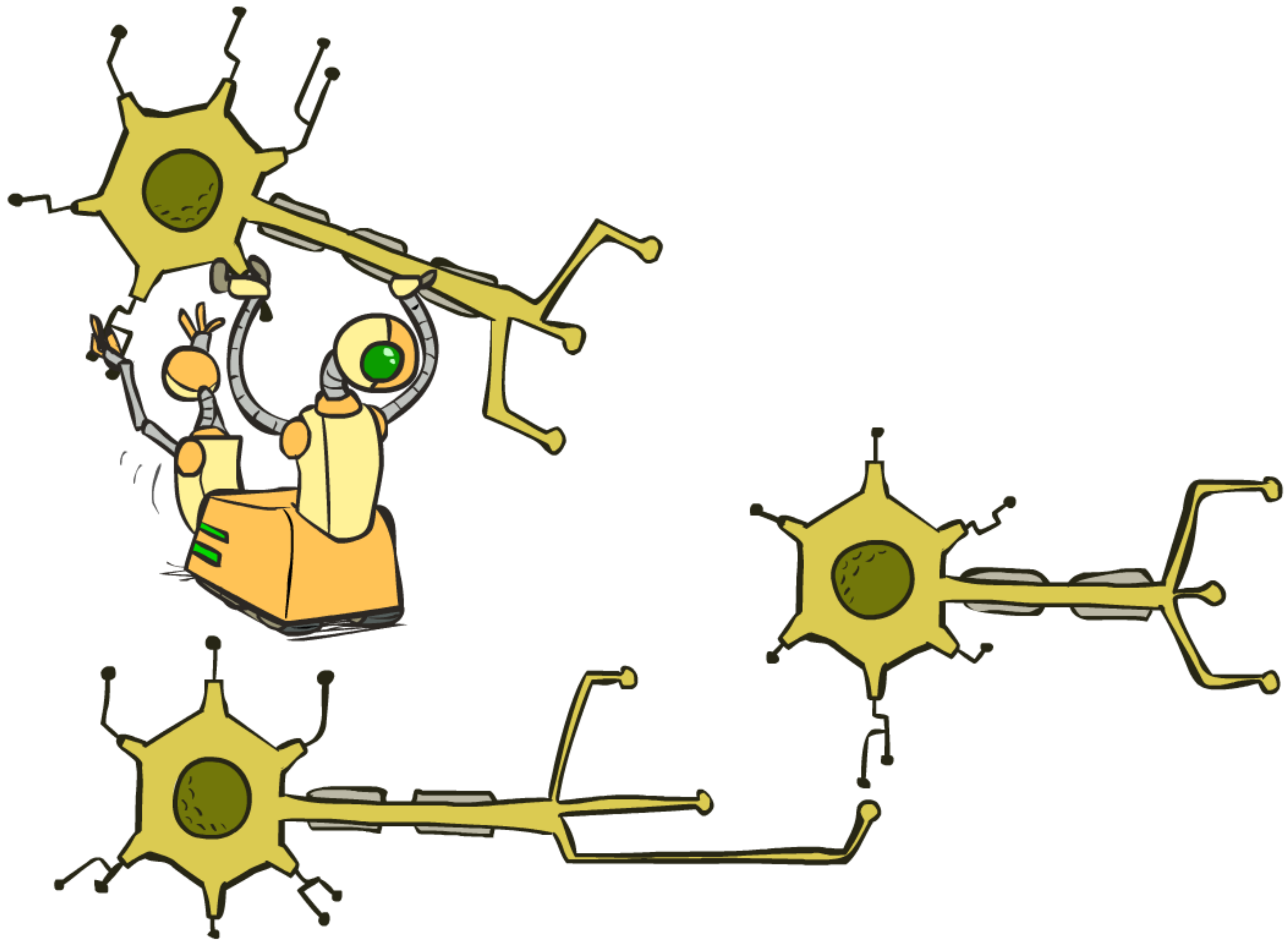
Supervised Machine Learning

AIMA Chapter 18, 20

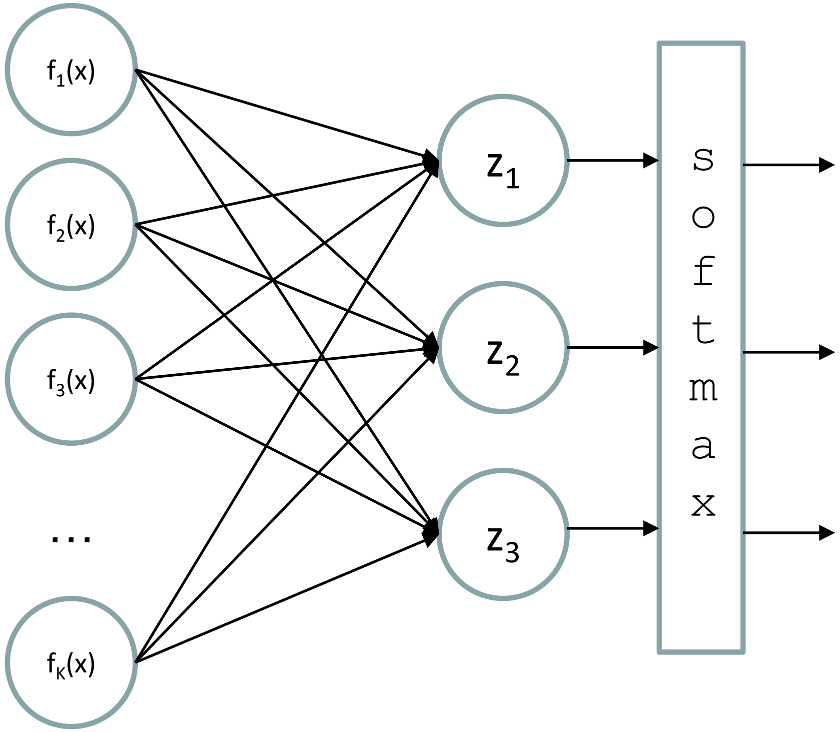
[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley]

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

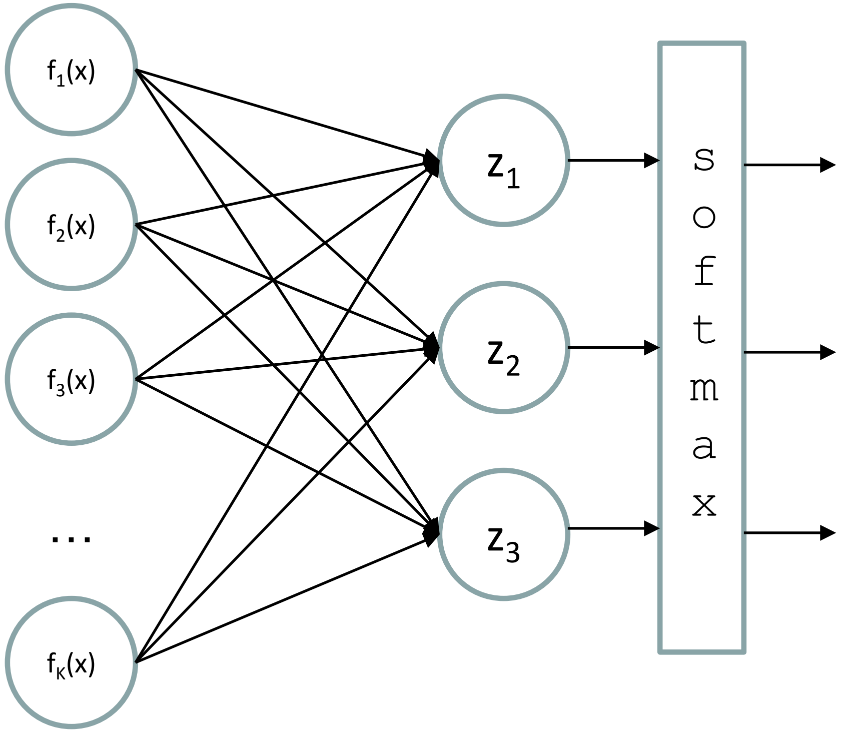


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

Deep Neural Network = Also learn the features!



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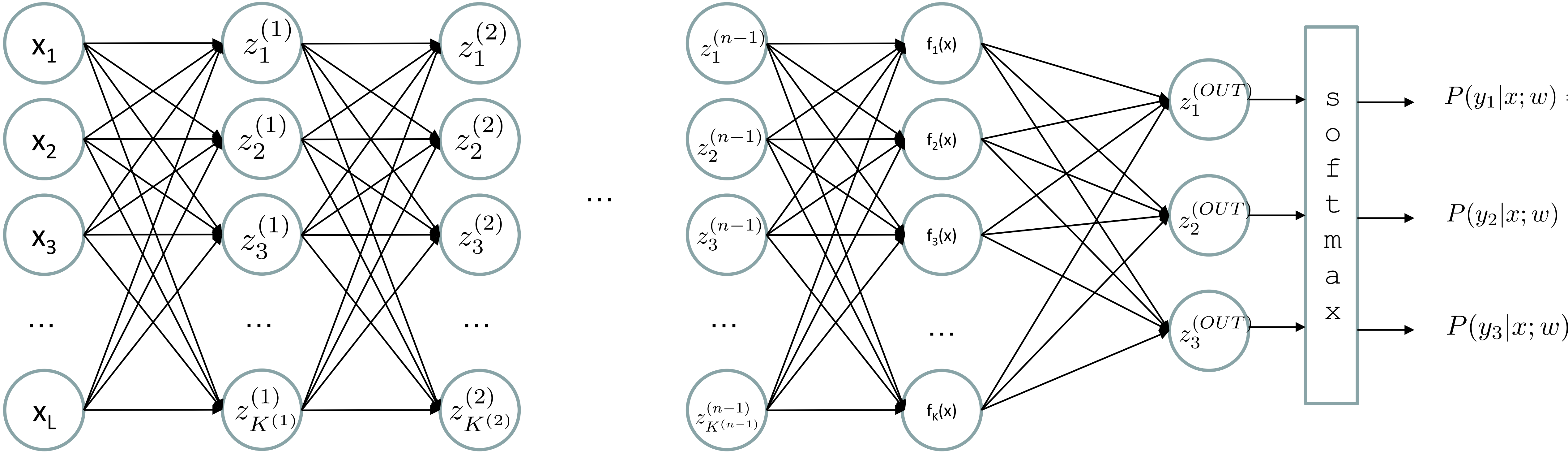
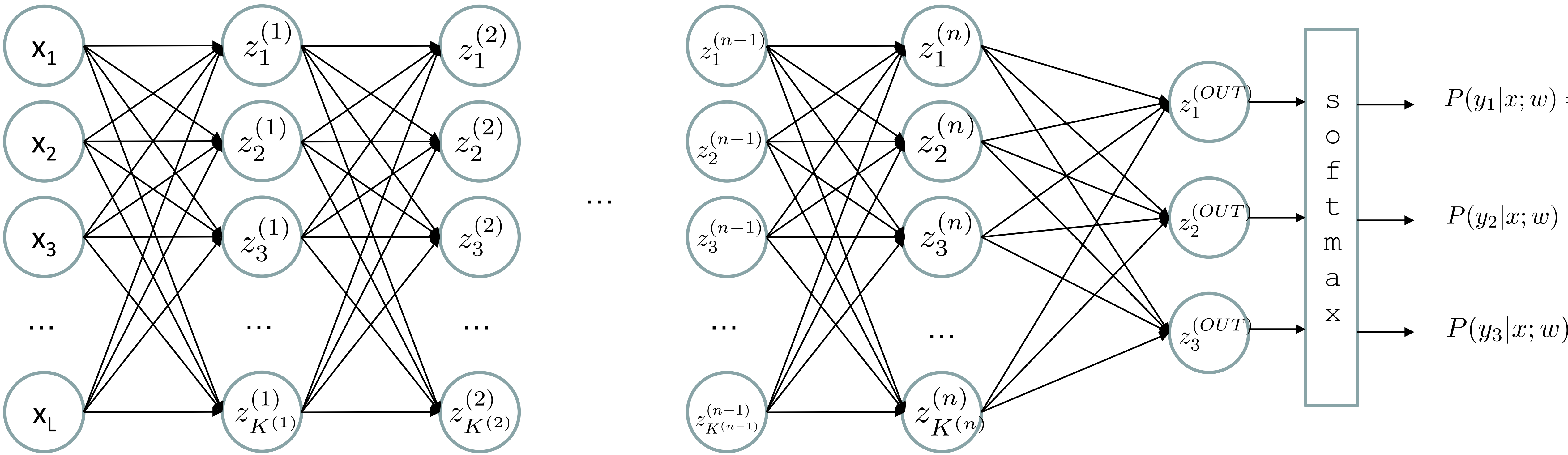


$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

g = nonlinear activation function

Deep Neural Network = Also learn the features!



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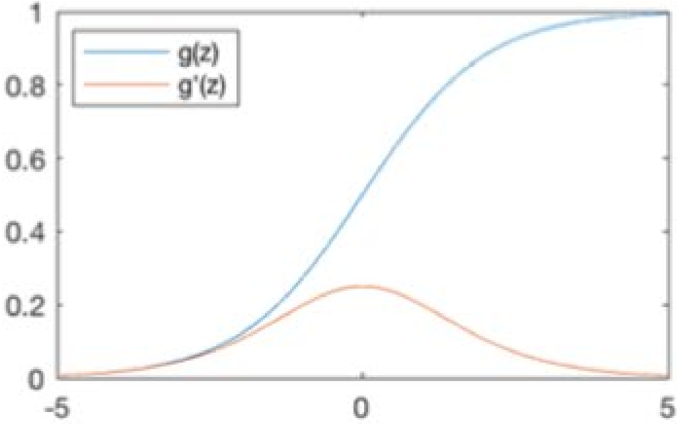
Common Activation Functions

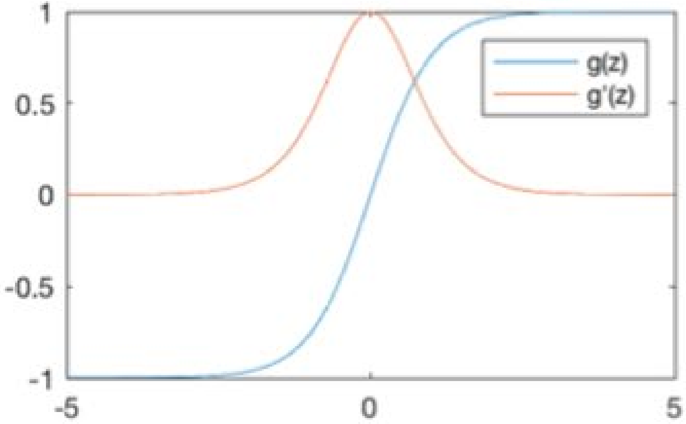
Sigmoid Function



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

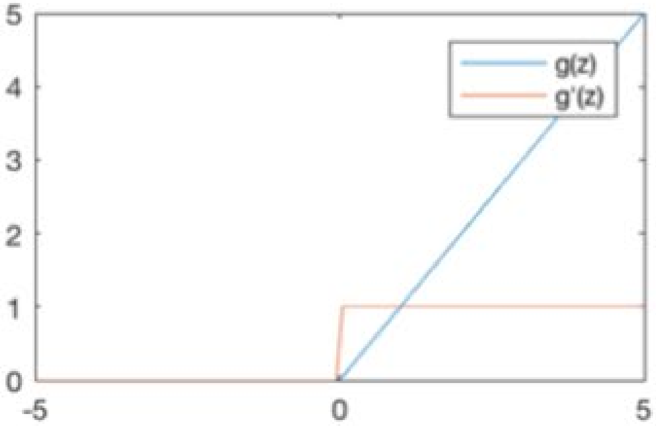
Hyperbolic Tangent



$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

[source: MIT 6.S191 introtodeeplearning.com]

Deep Neural Network: Also Learn the Features!

- Training the deep neural network is just like logistic regression:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

just w tends to be a much, much larger vector ☺

→just run gradient ascent

+ stop when log likelihood of hold-out data starts to decrease

Neural Networks Properties

- Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.

- Practical considerations
  - Can be seen as learning the features
  - Large number of neurons
    - Danger for overfitting
    - (hence early stopping!)

How about computing all the derivatives?

- Derivatives tables:

$$\frac{d}{dx}(a) = 0$$

$$\frac{d}{dx}(x) = 1$$

$$\frac{d}{dx}(au) = a\frac{du}{dx}$$

$$\frac{d}{dx}(u + v - w) = \frac{du}{dx} + \frac{dv}{dx} - \frac{dw}{dx}$$

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{u}{v}\right) = \frac{1}{v}\frac{du}{dx} - \frac{u}{v^2}\frac{dv}{dx}$$

$$\frac{d}{dx}(u^n) = nu^{n-1}\frac{du}{dx}$$

$$\frac{d}{dx}(\sqrt{u}) = \frac{1}{2\sqrt{u}}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u}\right) = -\frac{1}{u^2}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u^n}\right) = -\frac{n}{u^{n+1}}\frac{du}{dx}$$

$$\frac{d}{dx}[f(u)] = \frac{d}{du}[f(u)]\frac{du}{dx}$$

$$\frac{d}{dx}[\ln u] = \frac{d}{dx}[\log_e u] = \frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}[\log_a u] = \log_a e\frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}e^u = e^u\frac{du}{dx}$$

$$\frac{d}{dx}a^u = a^u \ln a\frac{du}{dx}$$

$$\frac{d}{dx}(u^v) = vu^{v-1}\frac{du}{dx} + \ln u \;\; u^v\frac{dv}{dx}$$

$$\frac{d}{dx}\sin u = \cos u\frac{du}{dx}$$

$$\frac{d}{dx}\cos u = -\sin u\frac{du}{dx}$$

$$\frac{d}{dx}\tan u = \sec^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\cot u = -\csc^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\sec u = \sec u \tan u\frac{du}{dx}$$

$$\frac{d}{dx}\csc u = -\csc u \cot u\frac{du}{dx}$$

[source: http://hyperphysics.phy-astr.gsu.edu/hbase/Math/derfunc.html

How about computing all the derivatives?

- But neural net f is never one of those?
  - No problem: CHAIN RULE:

If $$f(x) = g(h(x))$$

Then $$f'(x) = g'(h(x))h'(x)$$

→ **Derivatives can be computed by following well-defined procedures**

Automatic Differentiation

- Automatic differentiation software
  - e.g. PyTorch, TensorFlow, JAX
  - Only need to program the function g(x,y,w)
  - Can automatically compute all derivatives w.r.t. all entries in w
  - This is typically done by caching info during forward computation pass of f, and then doing a backward pass = “backpropagation”
  - Autodiff / Backpropagation can often be done at computational cost comparable to the forward pass
- Need to know this exists
- How this is done? -- outside of scope

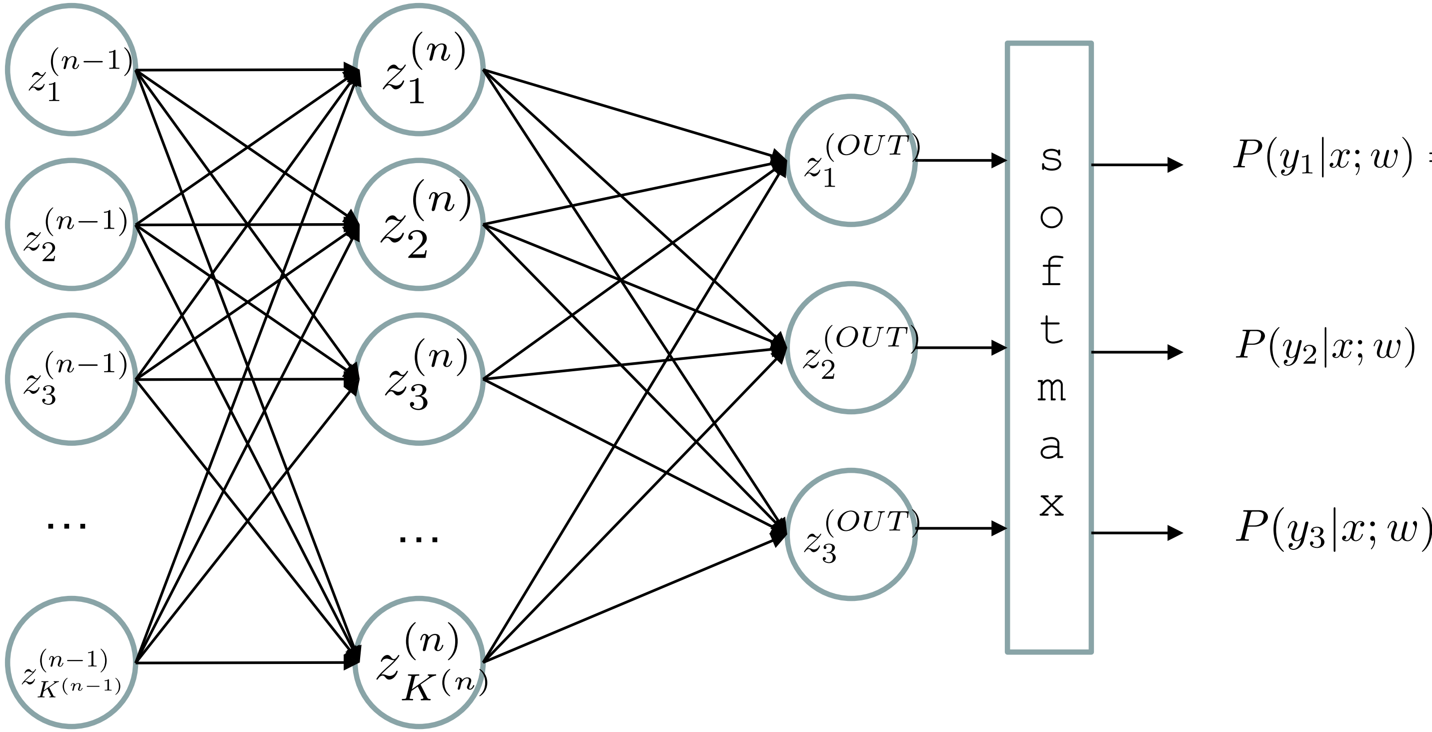
Summary of Key Ideas

- Optimize probability of label given input $\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$
- Continuous optimization
  - Gradient ascent:
    - Compute steepest uphill direction = gradient (= just vector of partial derivatives)
    - Take step in the gradient direction
    - Repeat (until held-out data accuracy starts to drop = "early stopping")
- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Universal function approximation theorem
    - `If` neural net is large enough
    - `Then` neural net can represent any continuous mapping from input to output with arbitrary accuracy
    - But remember: need to avoid overfitting / memorizing the training data → early stopping!
  - Automatic differentiation gives the derivatives efficiently (how? = outside of scope of 188)

Training a Network

Key words:

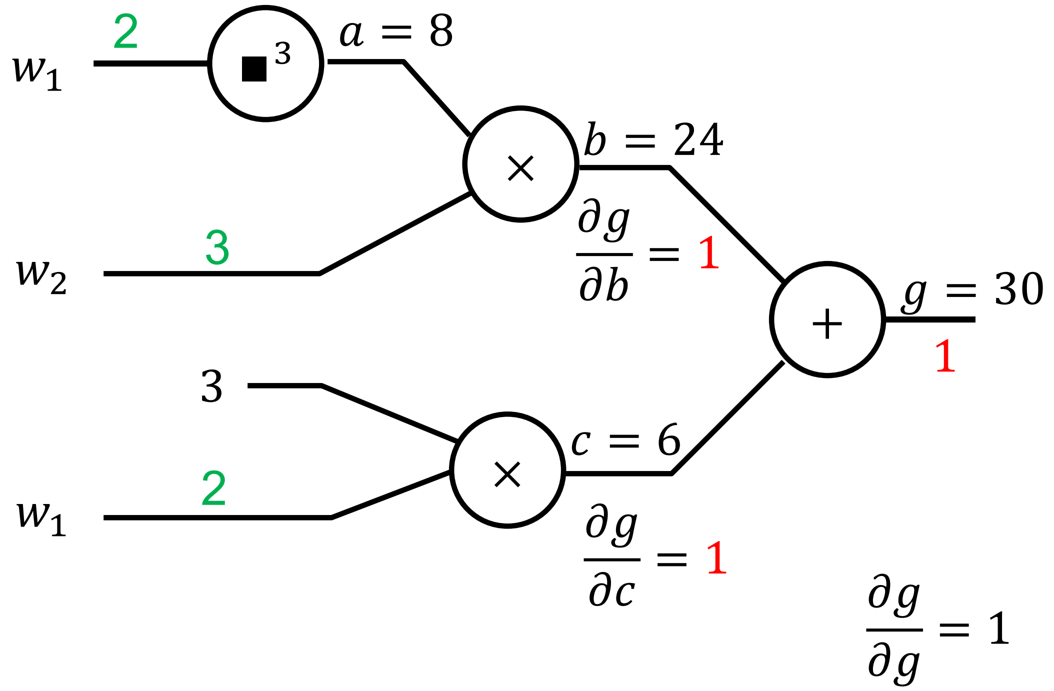
- Forward
- Backwards
- Gradient
- Backprop



g = nonlinear activation function

Back Propagation: $g(\boldsymbol{w}) = w_1^3 w_2 + 3w_1$

- Suppose we have $g(\boldsymbol{w}) = w_1^3 w_2 + 3w_1$ and want the gradient at $\boldsymbol{w} = [2, 3]$
- Think of the function as a composition of many functions.
  - Can use derivative chain rule to compute $\partial g / \partial w_1$ and $\partial g / \partial w_2$.
- $g = b + c$
  - $\frac{\partial g}{\partial b} = 1, \frac{\partial g}{\partial c} = 1$



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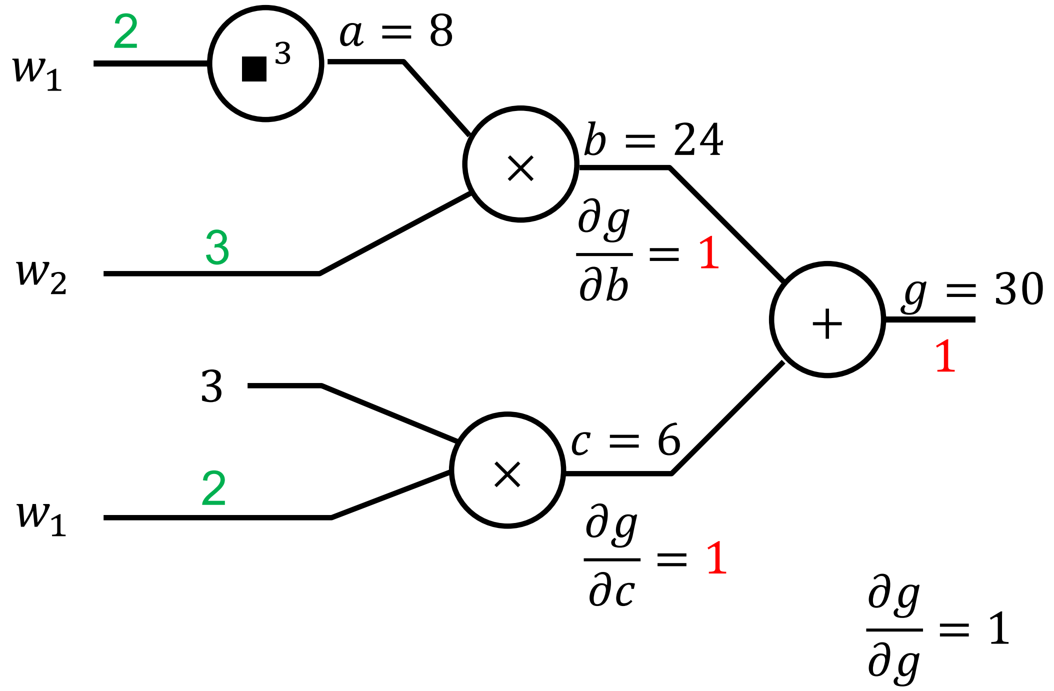

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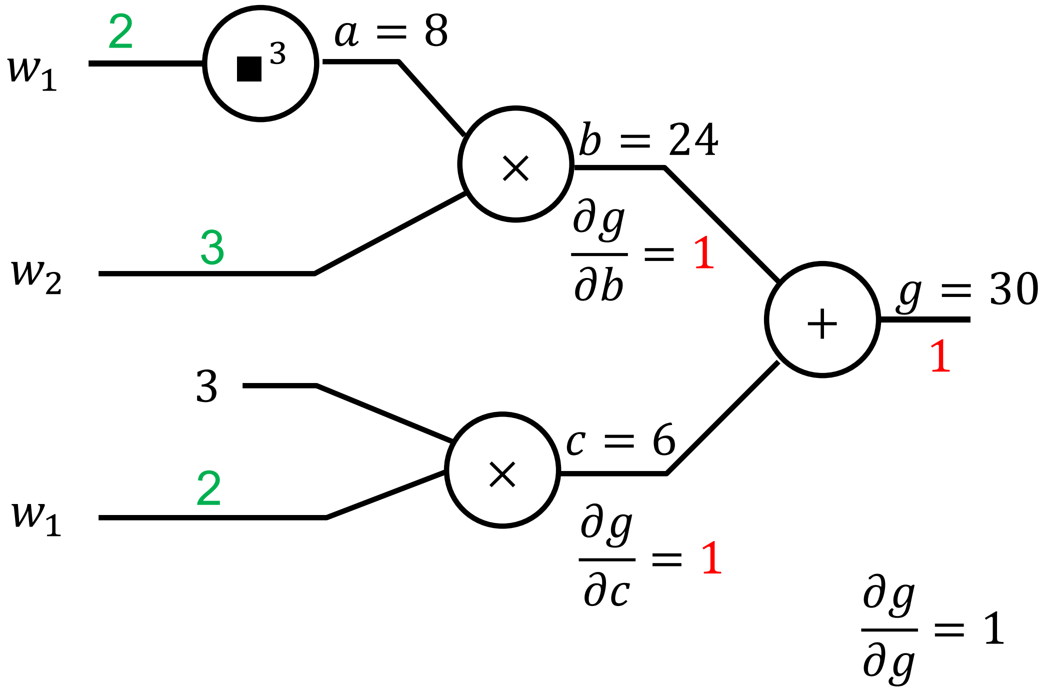

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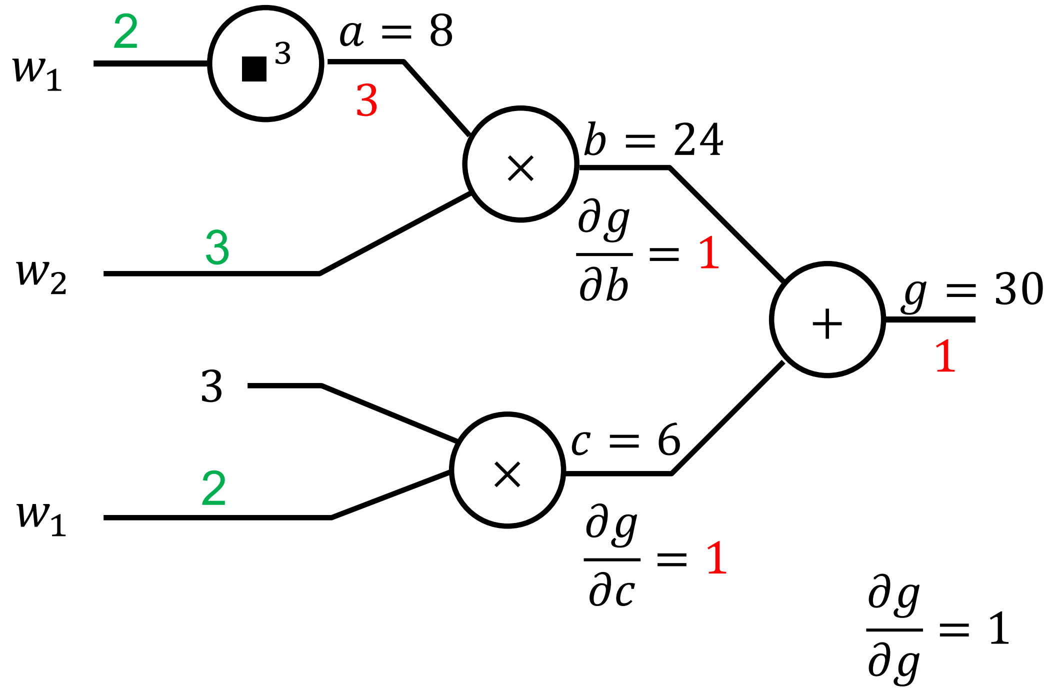

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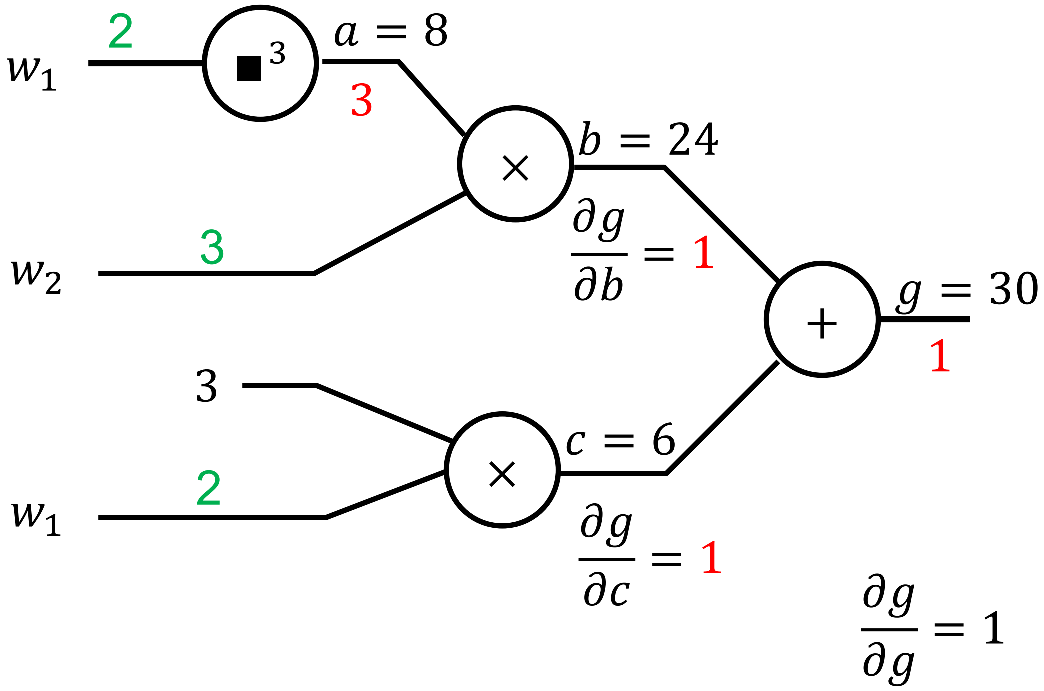

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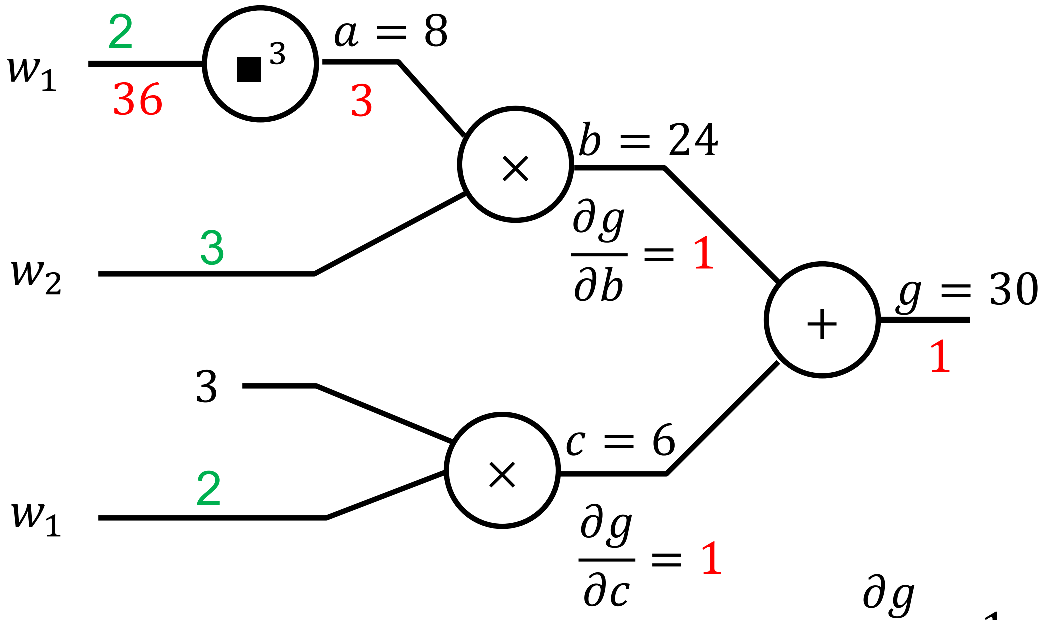

$\frac{\partial g}{\partial g} = 1$

Interpretation: A tiny increase in w_1 will result in an approximately $36w_1$ increase in g due to this cube function.

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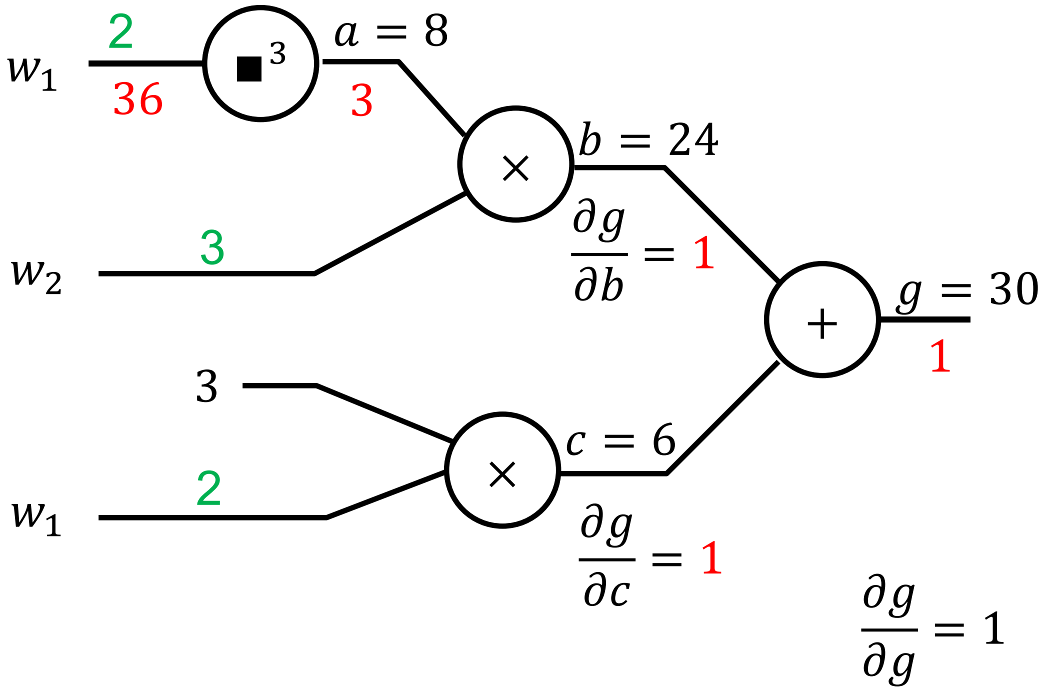
- $\frac{\partial g}{\partial w_2} = ???$

Hint: $b = a \times 3$ may be useful.



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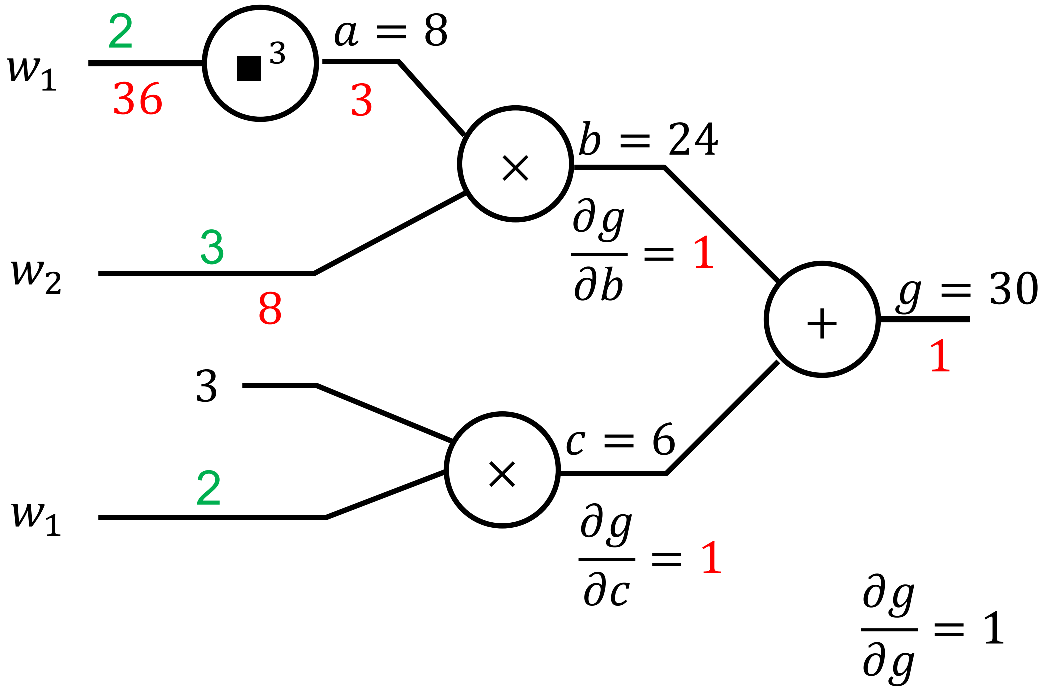

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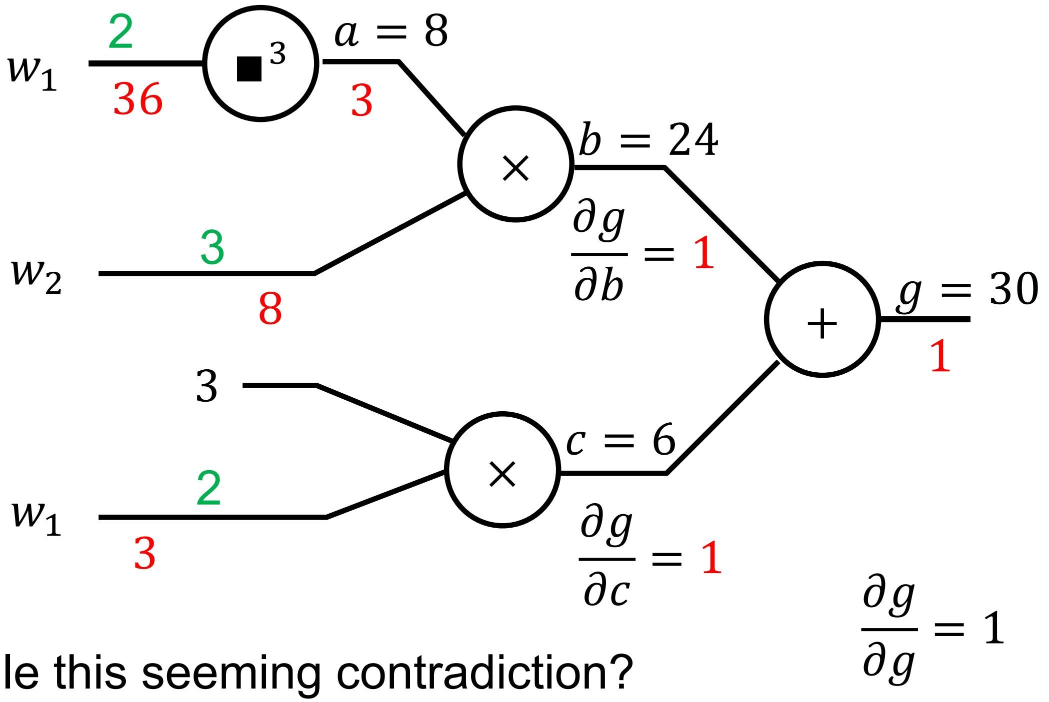

How do we reconcile this seeming contradiction? Top partial derivative means cube function contributes $36w_1$ and bottom p.d. means product contributes $3w_1$ so add them.

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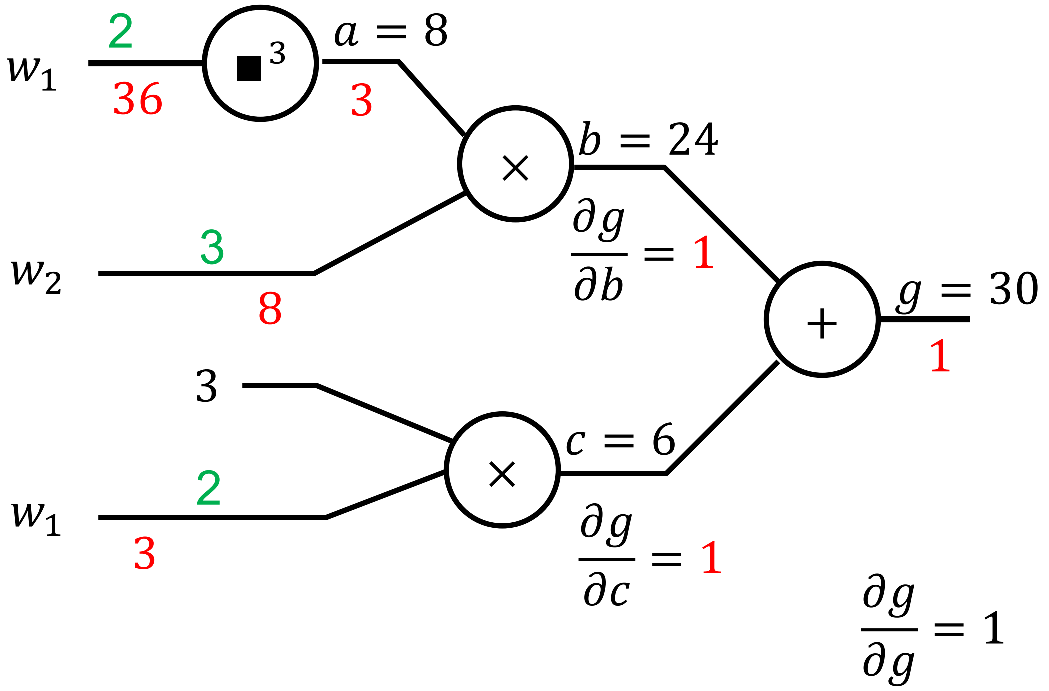


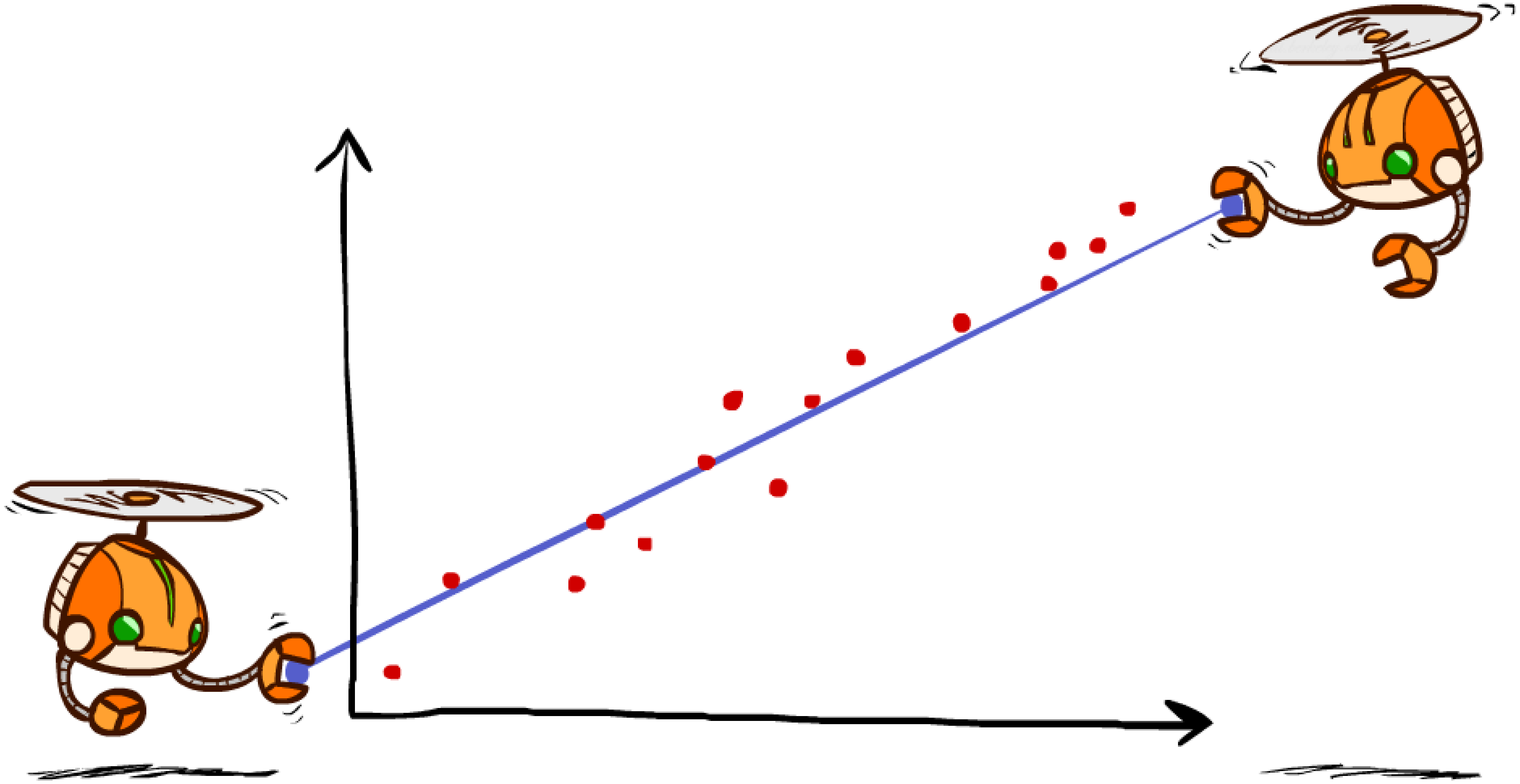
$$\nabla g = \left[\frac{\partial g}{\partial w_1}, \frac{\partial g}{\partial w_2}\right] = [39, 8]$$

Gradient Descent

- Punchline: If we can somehow compute our gradient, we can use gradient descent.
- How do we compute the gradient?
  - Purely analytically.
    - Gives exact symbolic answer. Infeasible for functions of lots of parameters or input values.
  - Finite difference approximation.
    - Gives approximation, very easy to implement.
    - Runtime for ll: $O(NM)$, where N is the number of parameters, and M is number of data points.
  - Back propagation.
    - Gives exact answer, difficult to implement.
    - Runtime for ll: $O(NM)$

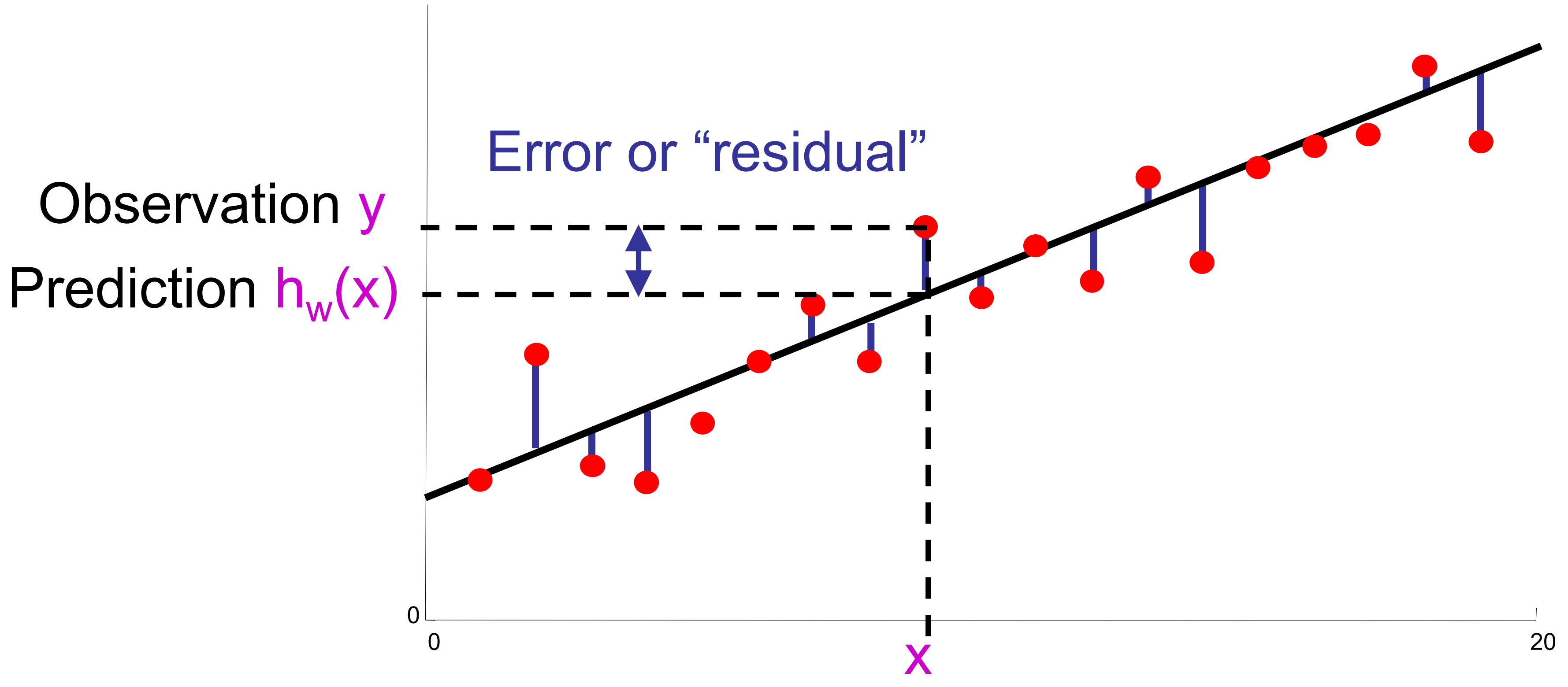
$$ll(w) = \sum_{i=1}^{m} \log p(y = y^{(i)} | f(x^{(i)}); w)$$

Regression



Linear Regression

Prediction: $h_w(x) = w_0 + w_1 x$



Error on one instance: $|y - h_w(x)|$

Least squares: Minimizing squared error

- L2 loss function: sum of squared errors over all examples

$$L(\boldsymbol{w}) = \sum_i \left(y_i - h_w(\boldsymbol{x}_i)\right)^2 = \sum_i (y_i - \boldsymbol{w}^T \boldsymbol{x}_i)^2$$

- We want the weights w* that minimize loss
- Analytical solution: at w* the derivative of loss w.r.t. each weight is zero
  - **X** is the data matrix (all the data, one example per row); **y** is the vector of labels
  - $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

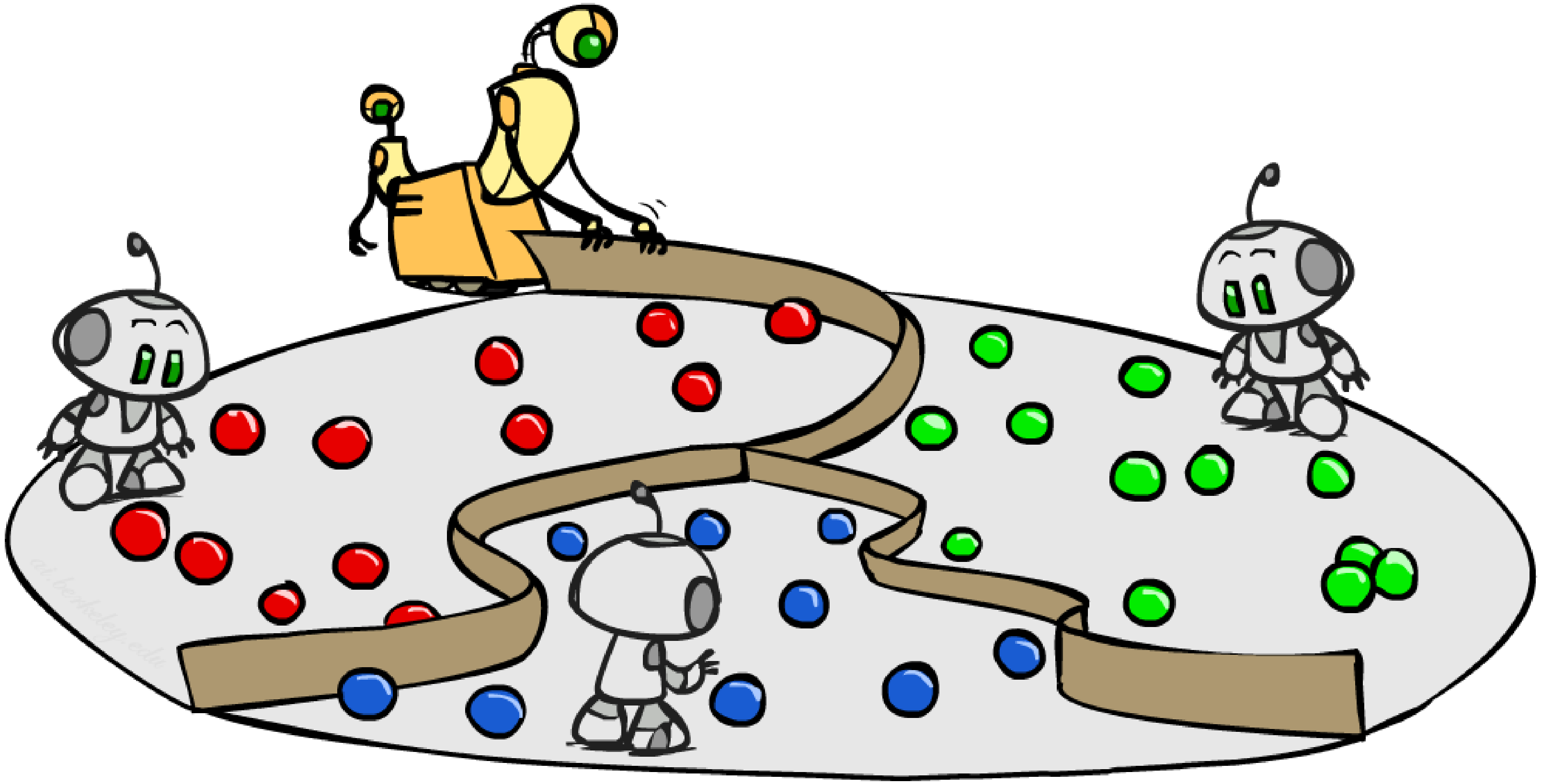
Non-linear least squares

- No closed-form solution in general
- Numerical algorithms are typically used
  - Choose initial values for the parameters and then refine the parameters iteratively
  - Gradient descent
  - Gauss–Newton method
  - Limited-memory BFGS
  - Derivative-free methods
  - etc.

Summary

- Supervised learning:
  - Learning a function from labeled examples
- Classification: discrete-valued function
  - Naïve Bayes
  - Generalization and overfitting, smoothing
  - Perceptron
- Regression: real-valued function
  - Linear regression

Unsupervised Machine Learning



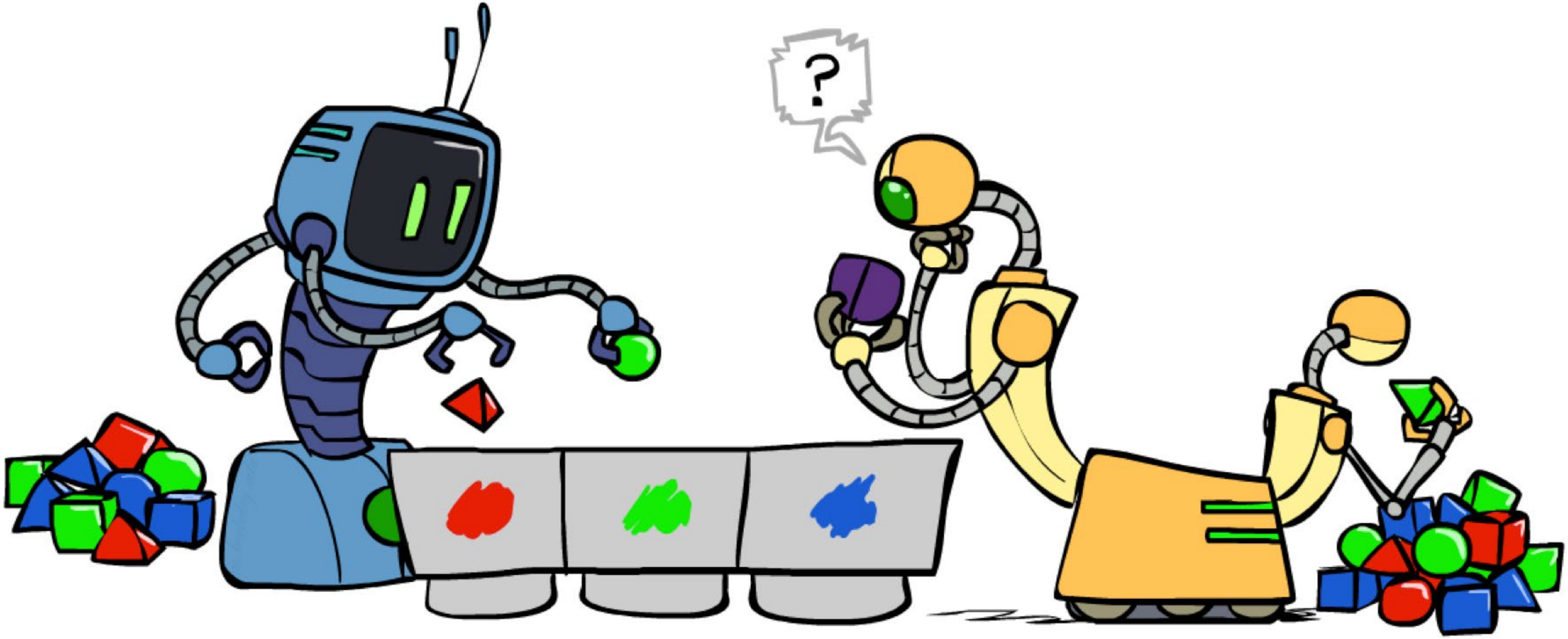
AIMA Chapter 20

[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley and from Daniel Weld, Carlos Guestrin, & Luke Zettlemoyer at U Washington]

Types of Learning

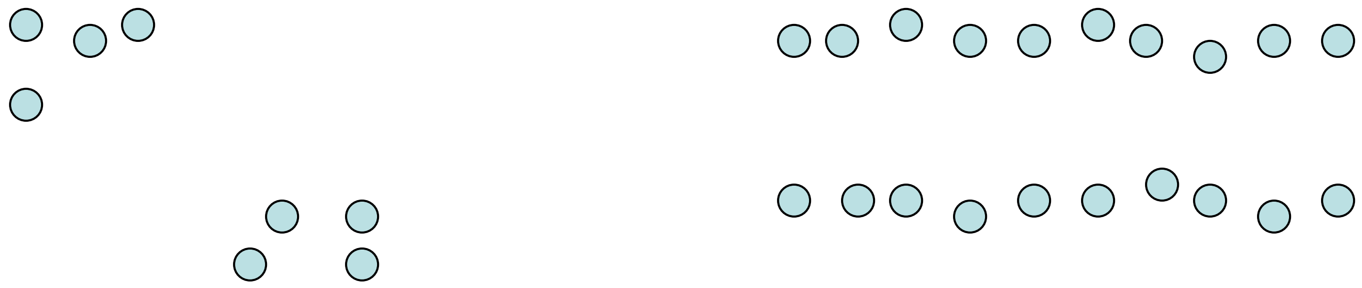
- Supervised learning
  - Training data includes desired outputs
- Unsupervised learning
  - Training data does not include desired outputs
- Semi-supervised learning
  - Training data includes a few desired outputs
- Reinforcement learning
  - Rewards from sequence of actions

Clustering



Clustering

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



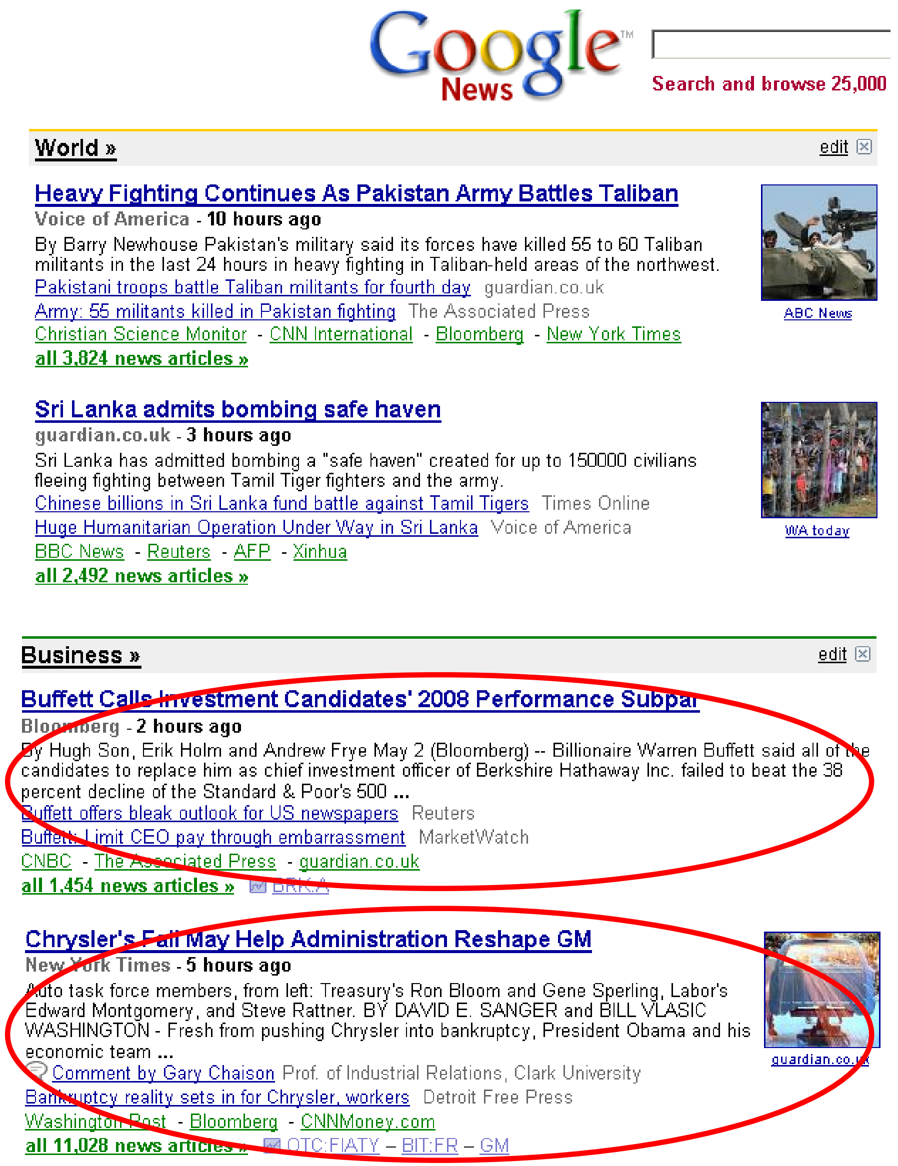
- What could "similar" mean?
  - One option: small (squared) Euclidean distance

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

  - Many other options, often domain specific

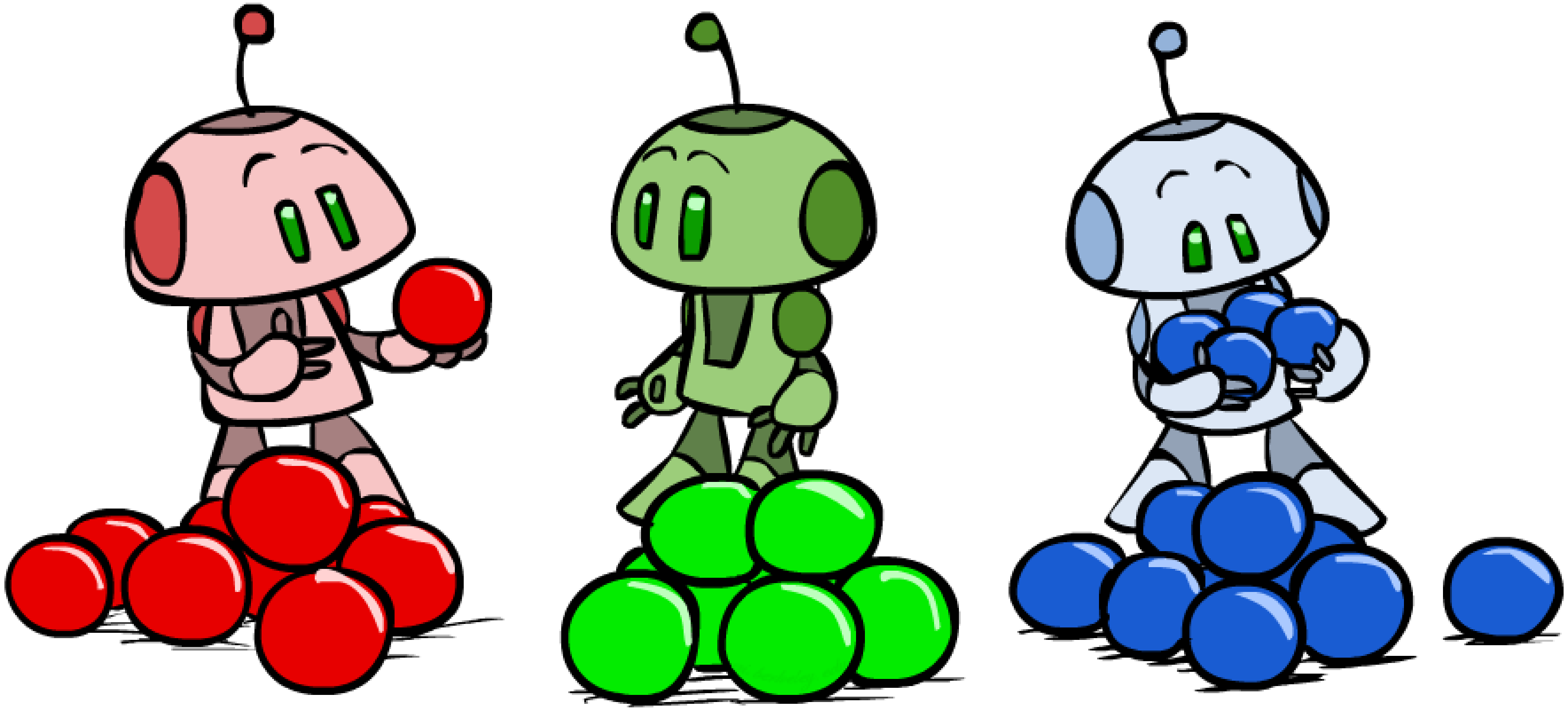
Clustering

- Applications
  - Group emails
  - Group search results
  - Find categories of customers
  - Detect anomalous program executions



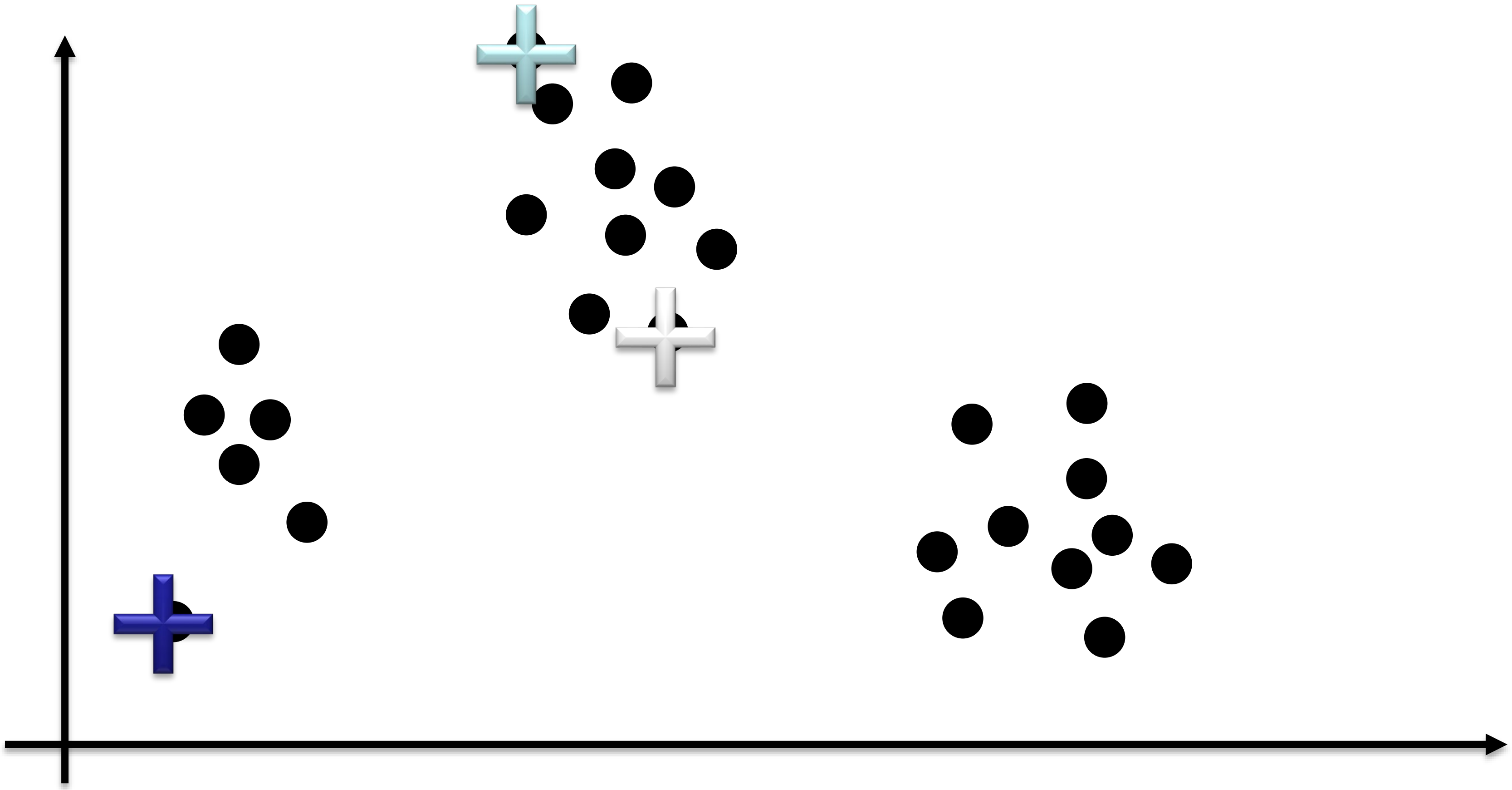
Story groupings: unsupervised clustering

K-Means



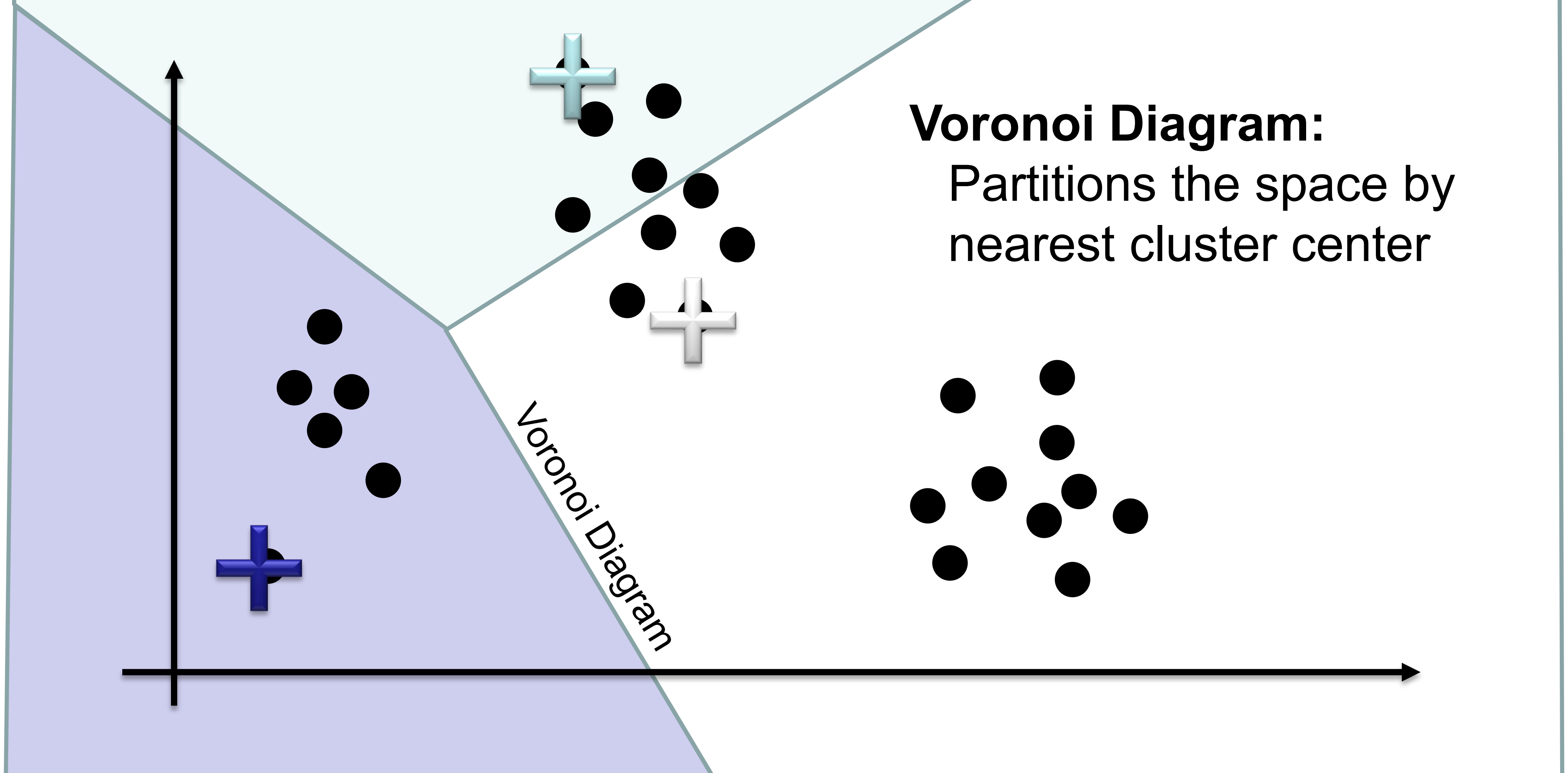
K-Means Clustering: *Intuition*

- Input K: The number of clusters to find
- Pick an initial set of points as cluster centers



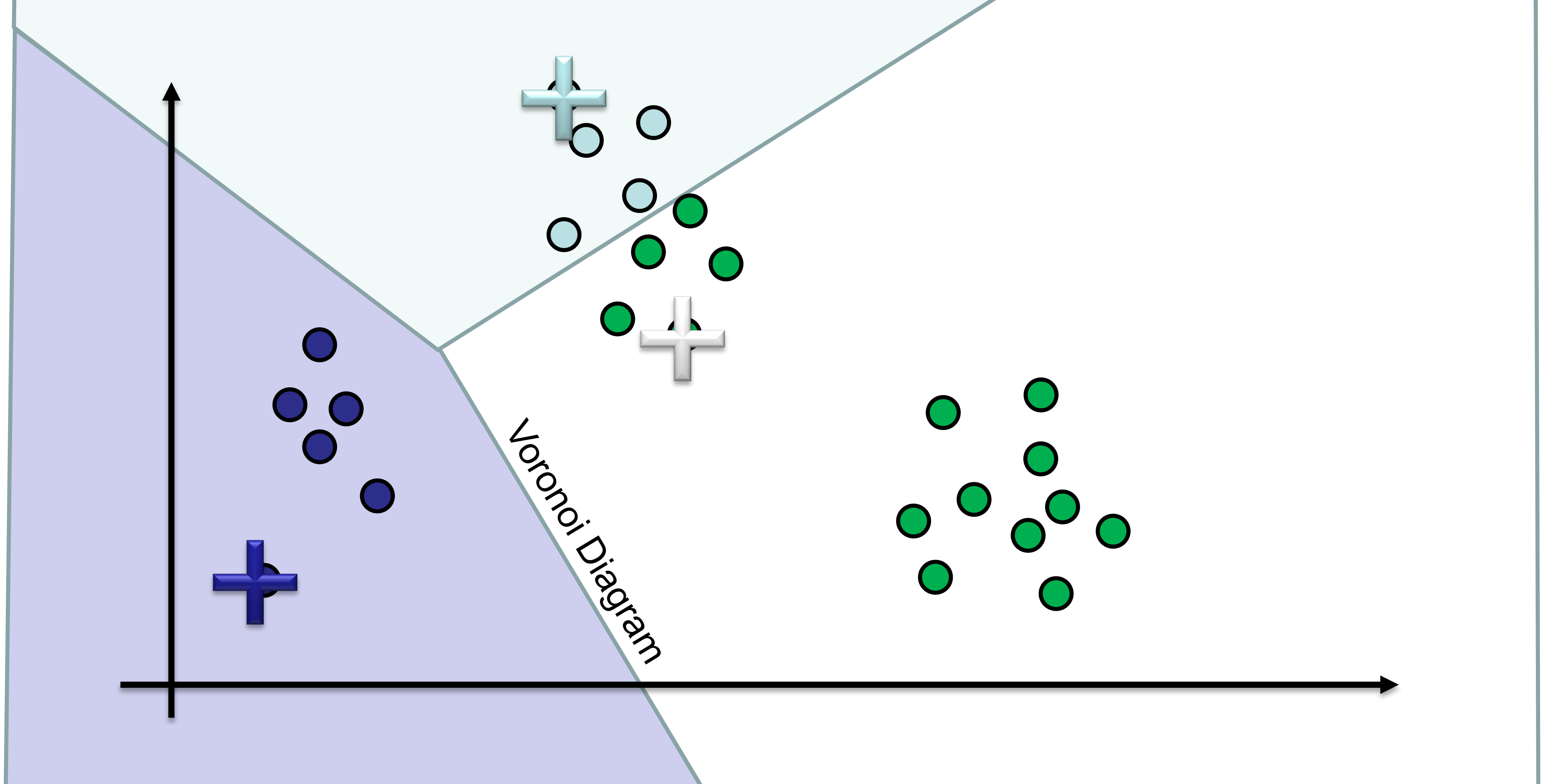
K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



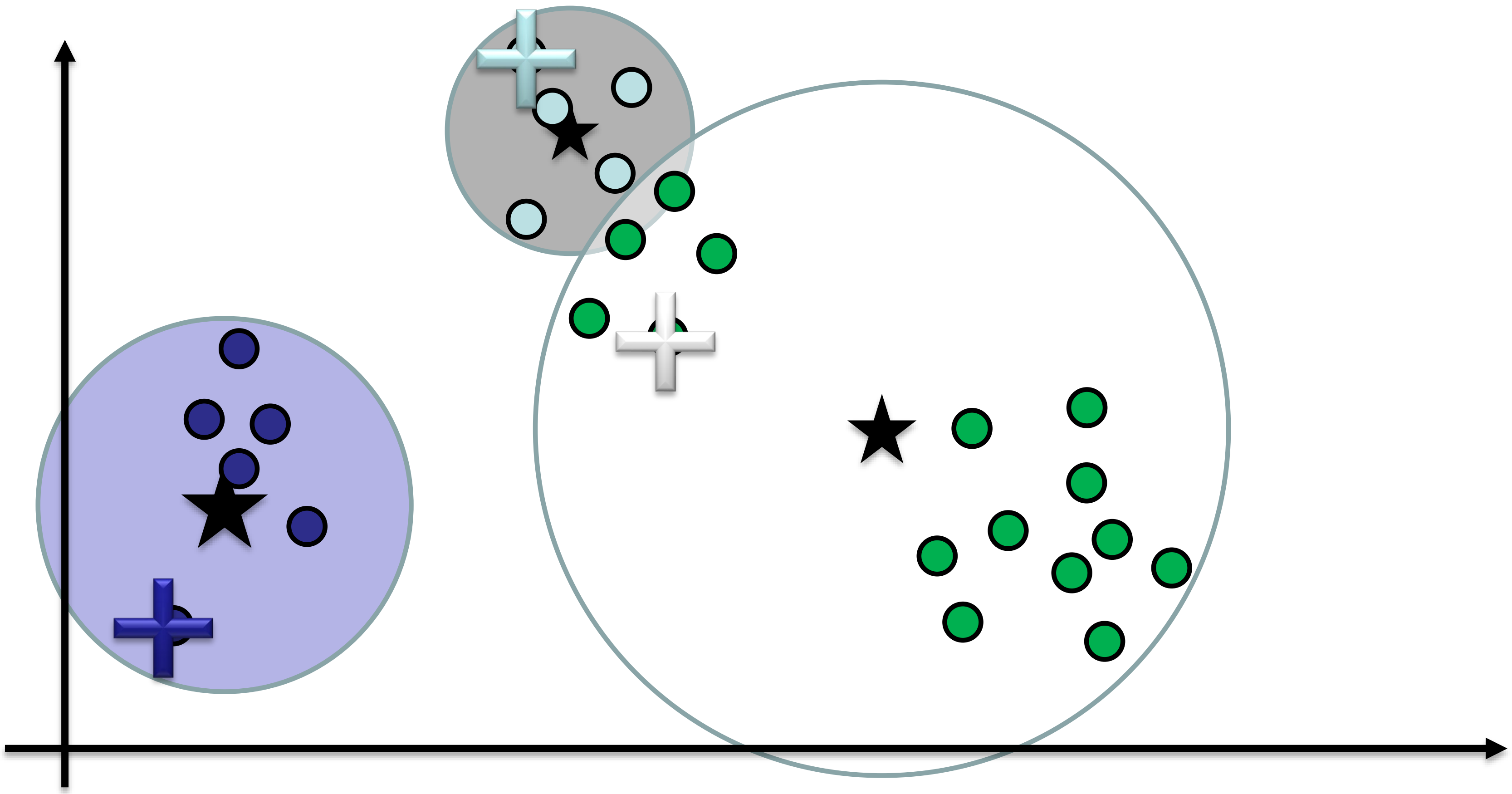
K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



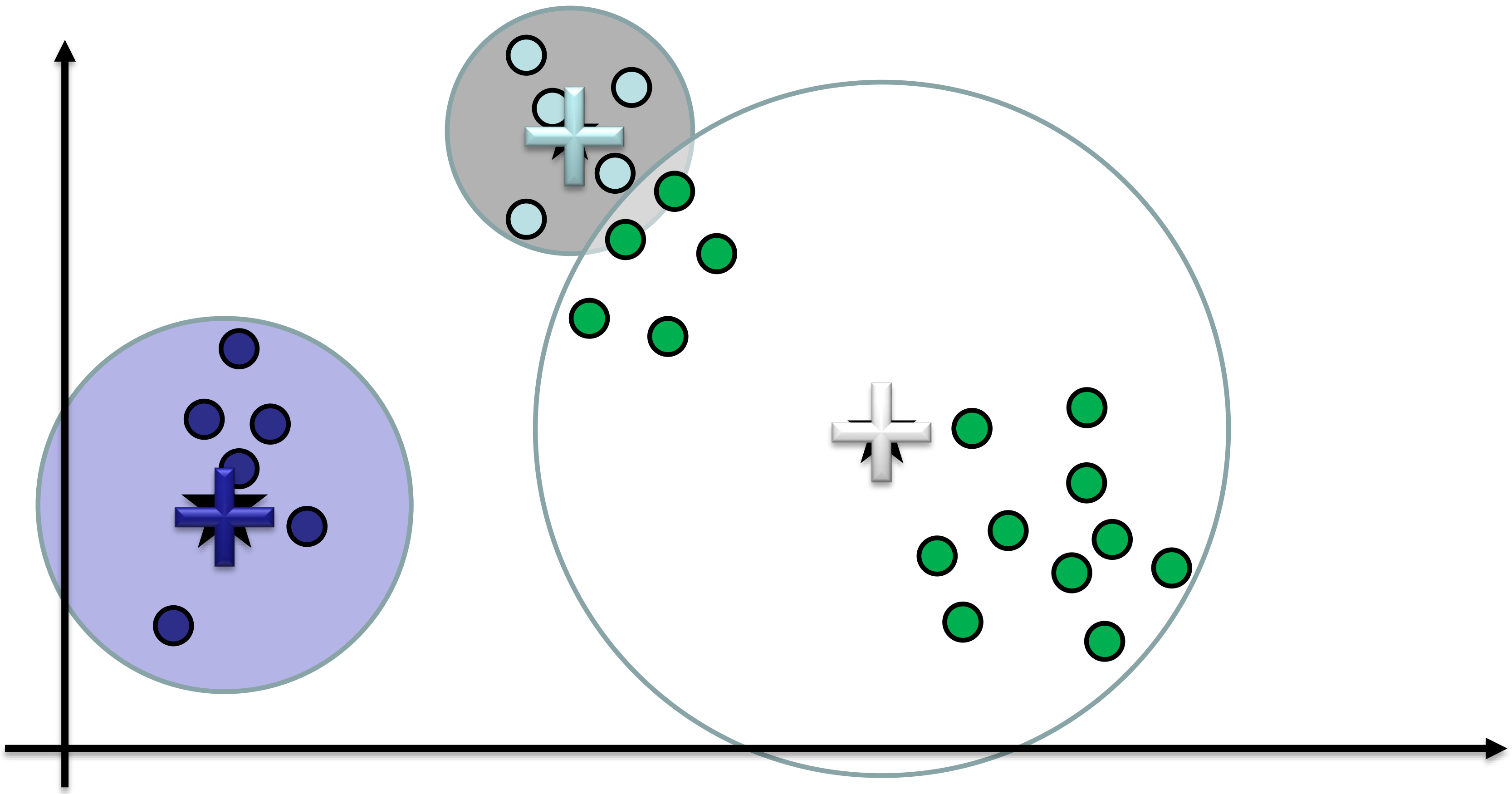
K-Means Clustering: *Intuition*

- Compute mean of points in each "cluster"



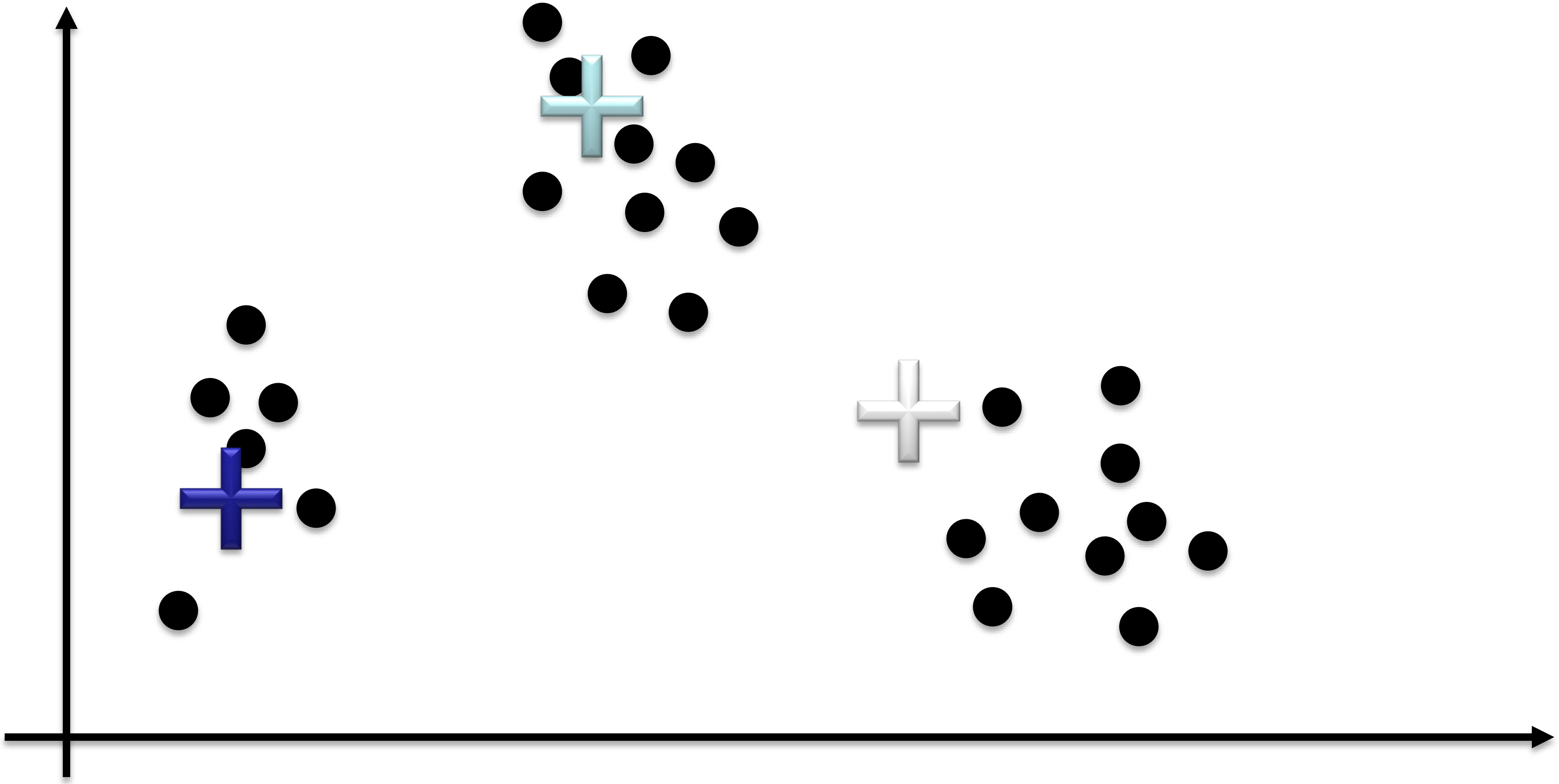
K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster



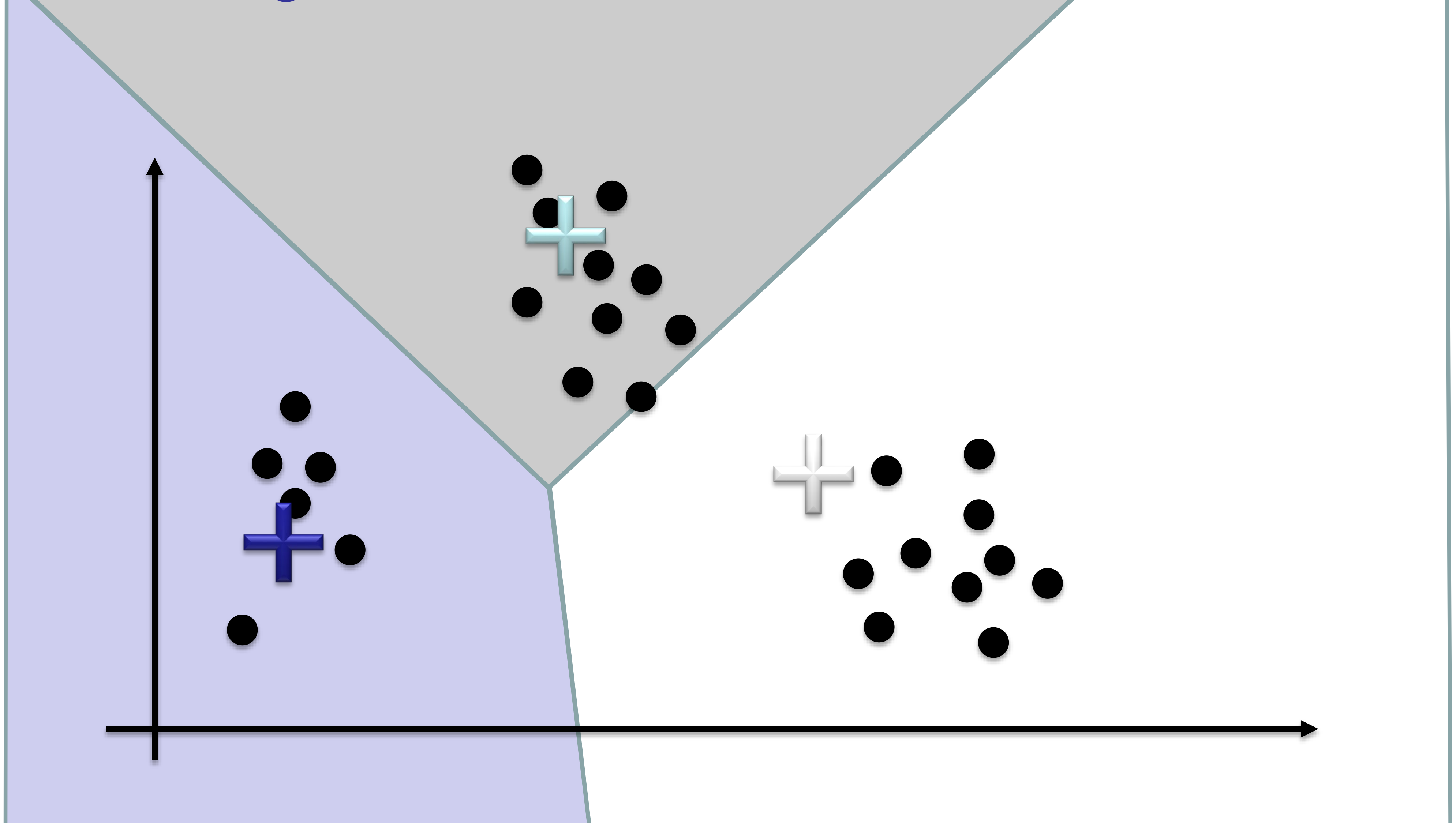
K-Means Clustering: *Intuition*

- Improved?
- Repeat



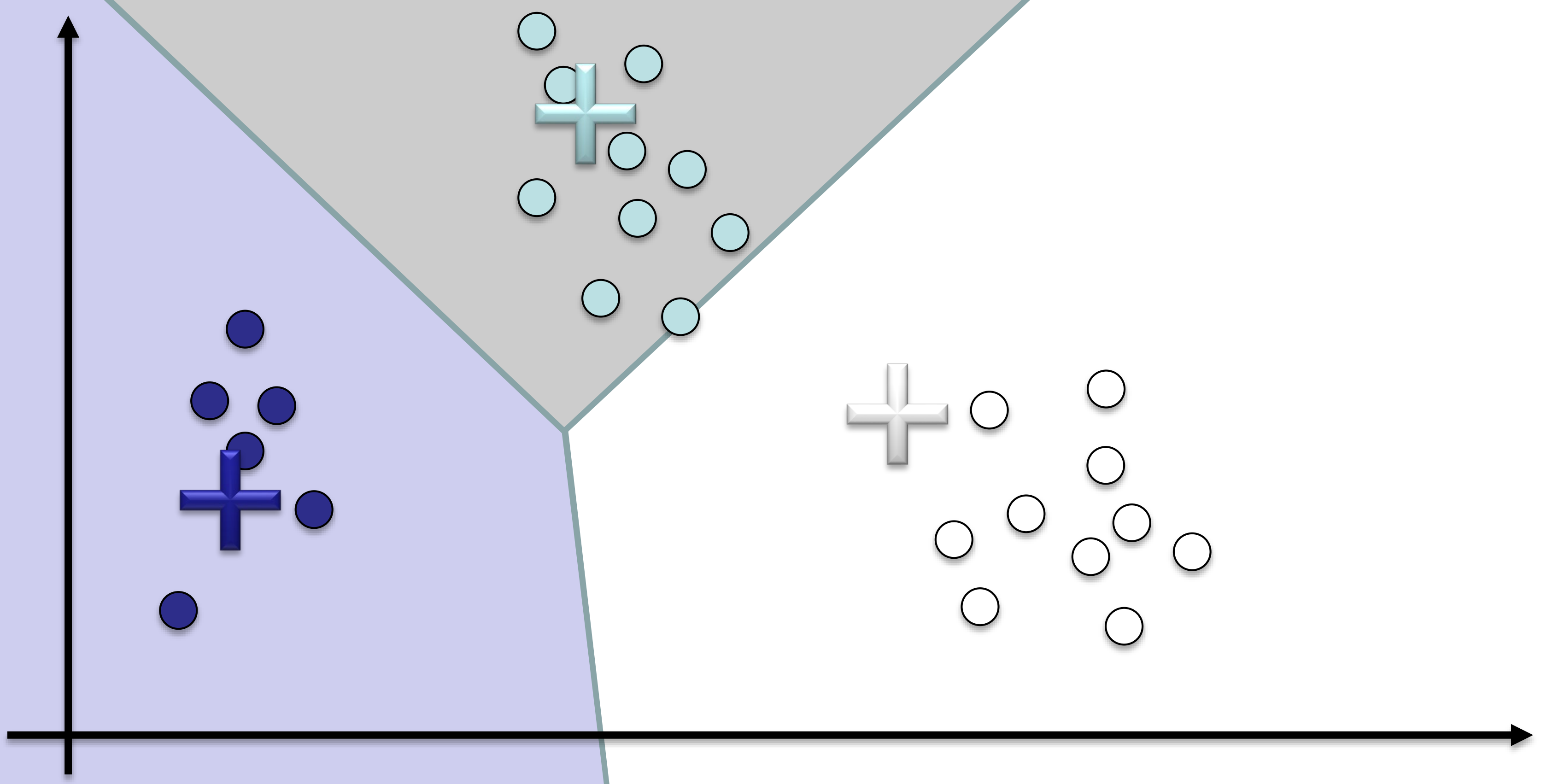
K-Means Clustering: *Intuition*

- Assign Points



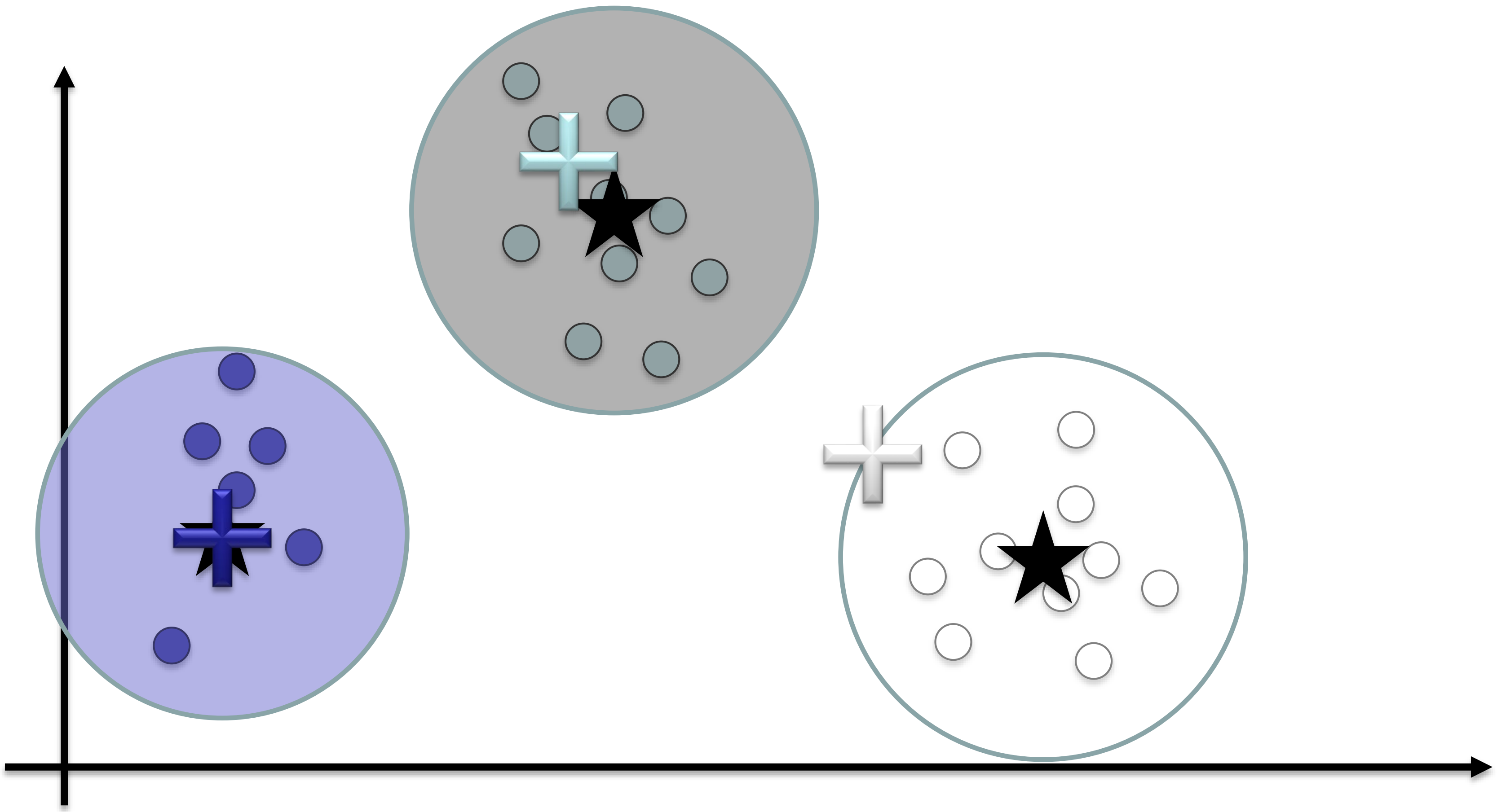
K-Means Clustering: *Intuition*

- Assign Points



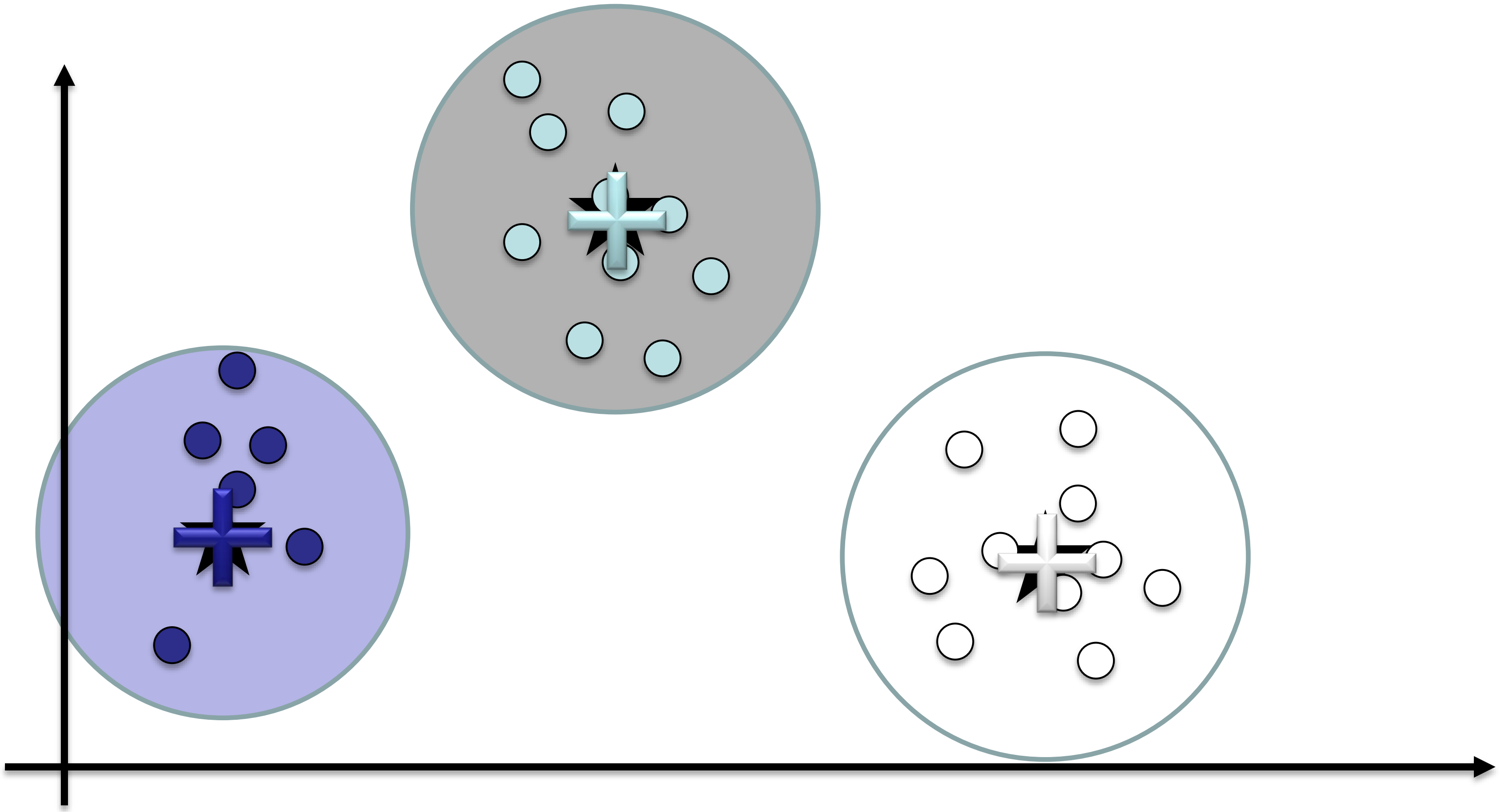
K-Means Clustering: *Intuition*

- Compute cluster means



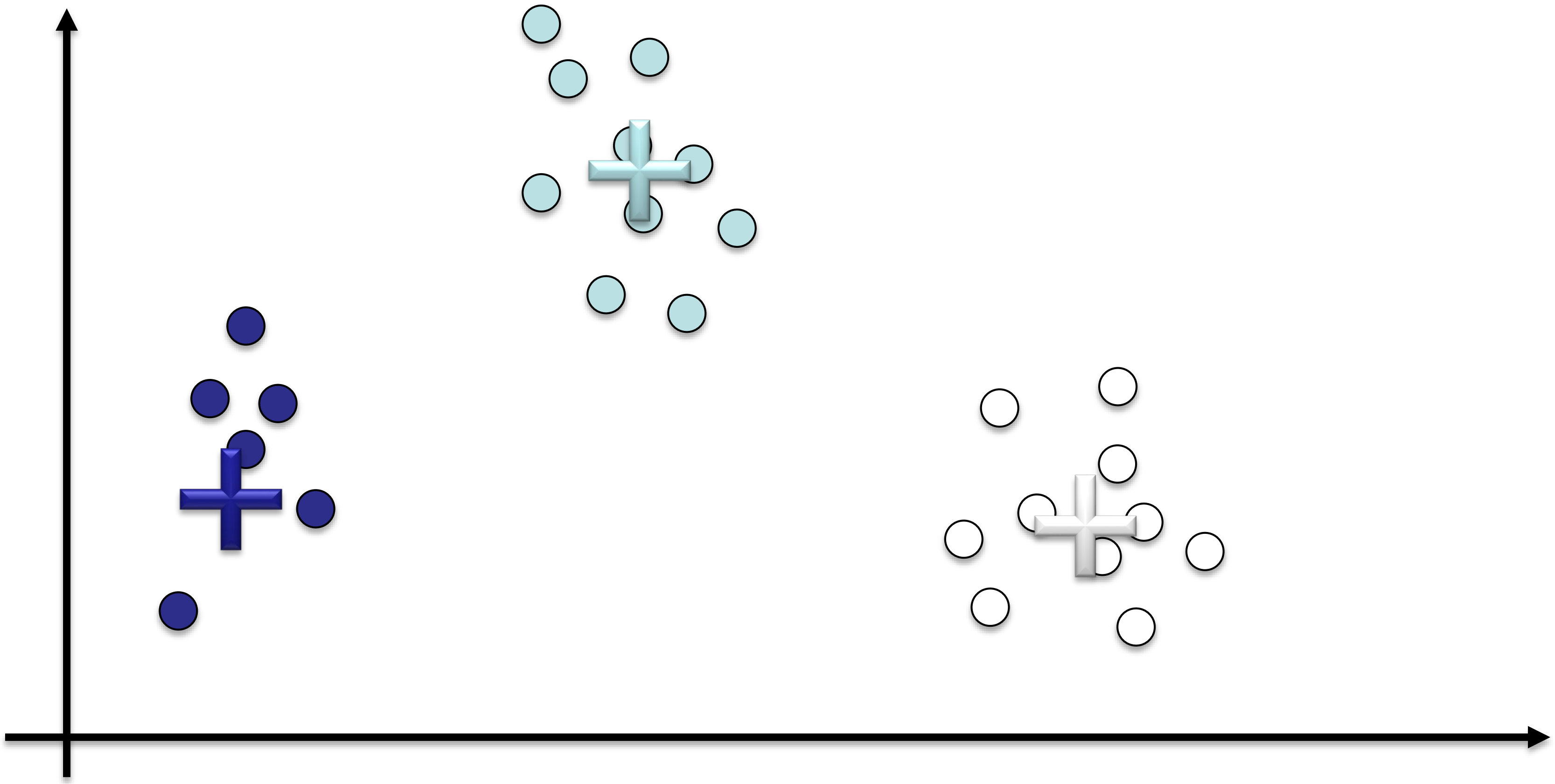
K-Means Clustering: *Intuition*

- Update cluster centers



K-Means Clustering: *Intuition*

- Repeat?
  - Yes to check that nothing changes → Converged!



K-Means as Optimization

- Consider the total distance to the means:

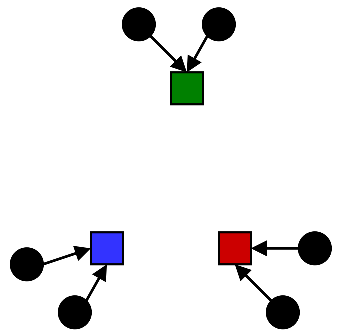
$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

points

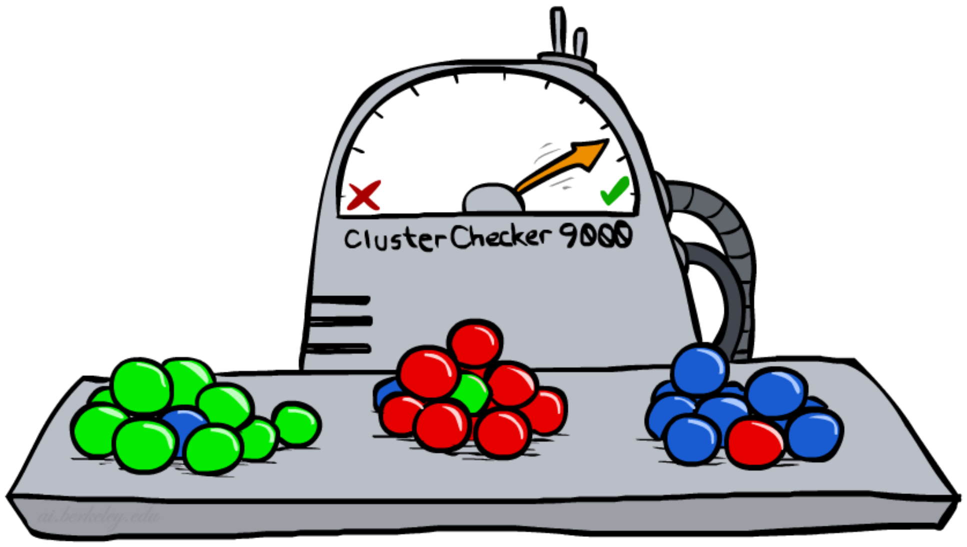
assignments

means

squared Euclidean distance



- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c
- Each step cannot increase phi



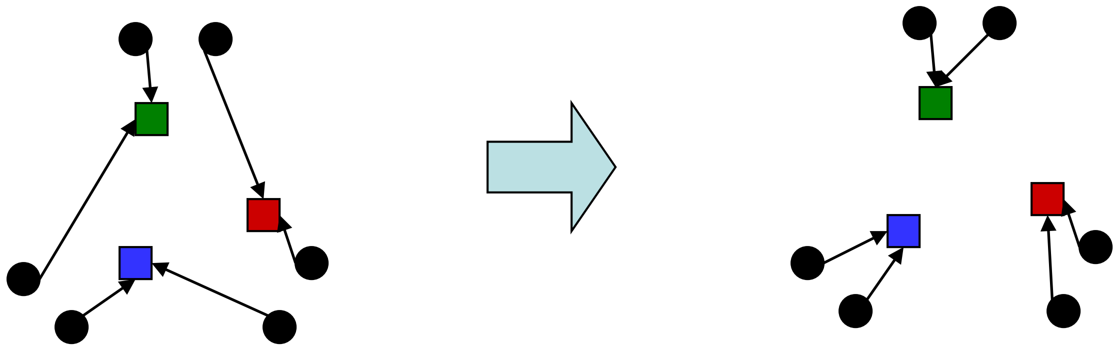
Phase I: Update Assignments

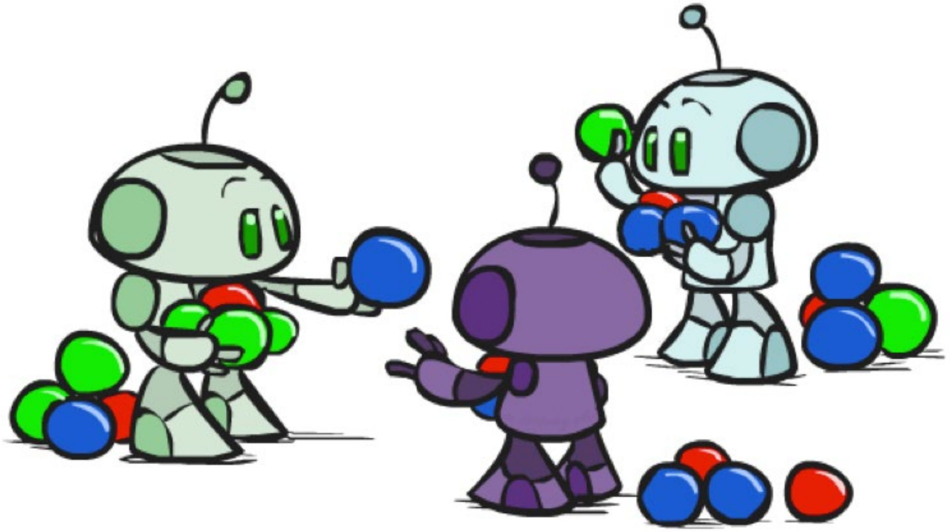
- For each point, re-assign to closest mean:

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

- Cannot increase total distance phi!

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

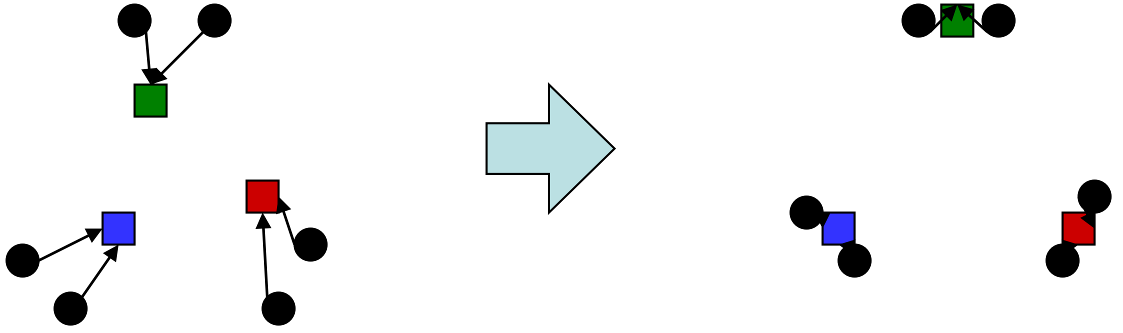




Phase II: Update Means

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

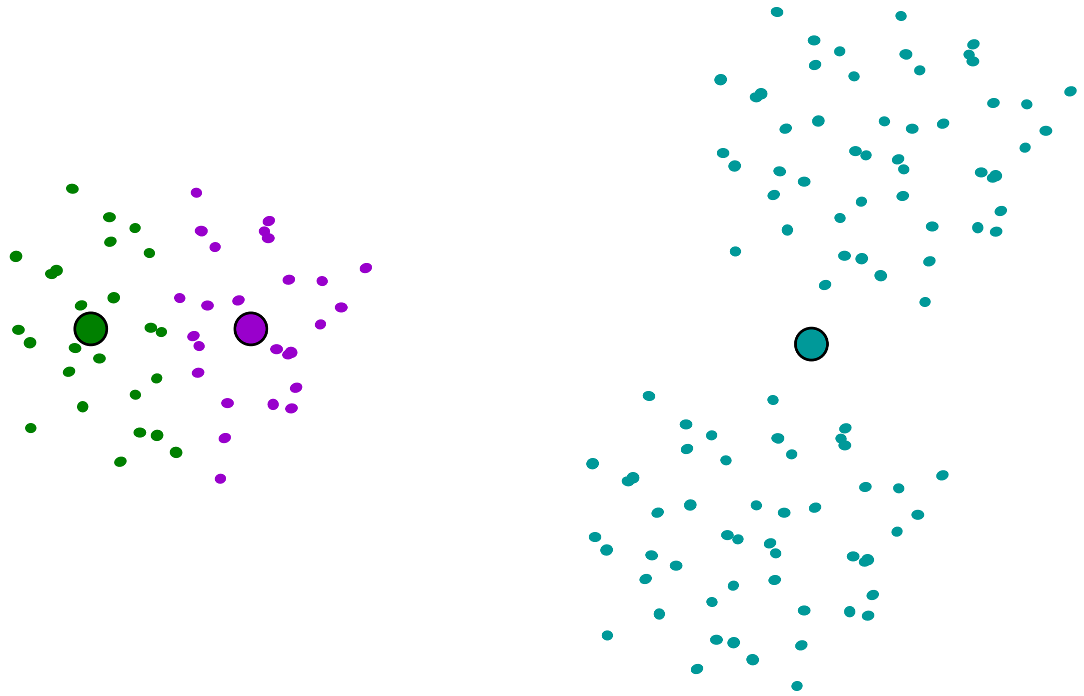
$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

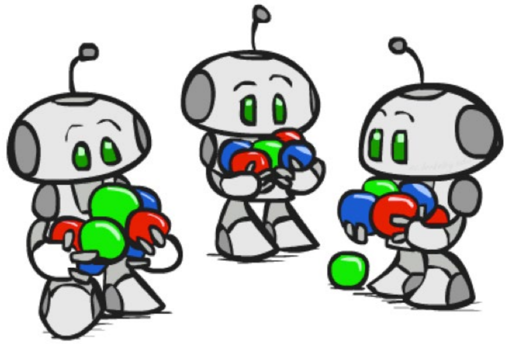


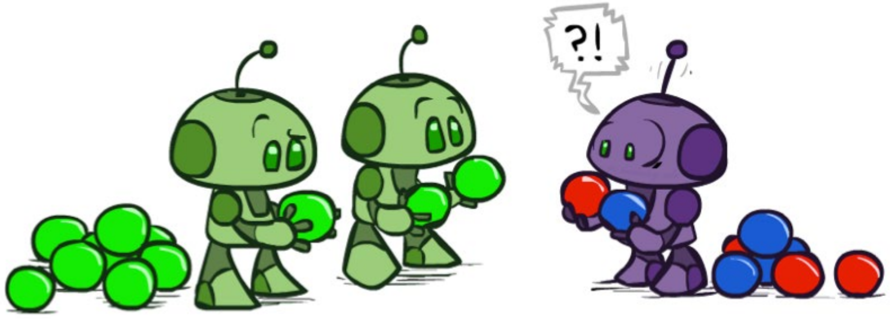
- Also cannot increase total distance
  - Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean

Initialization

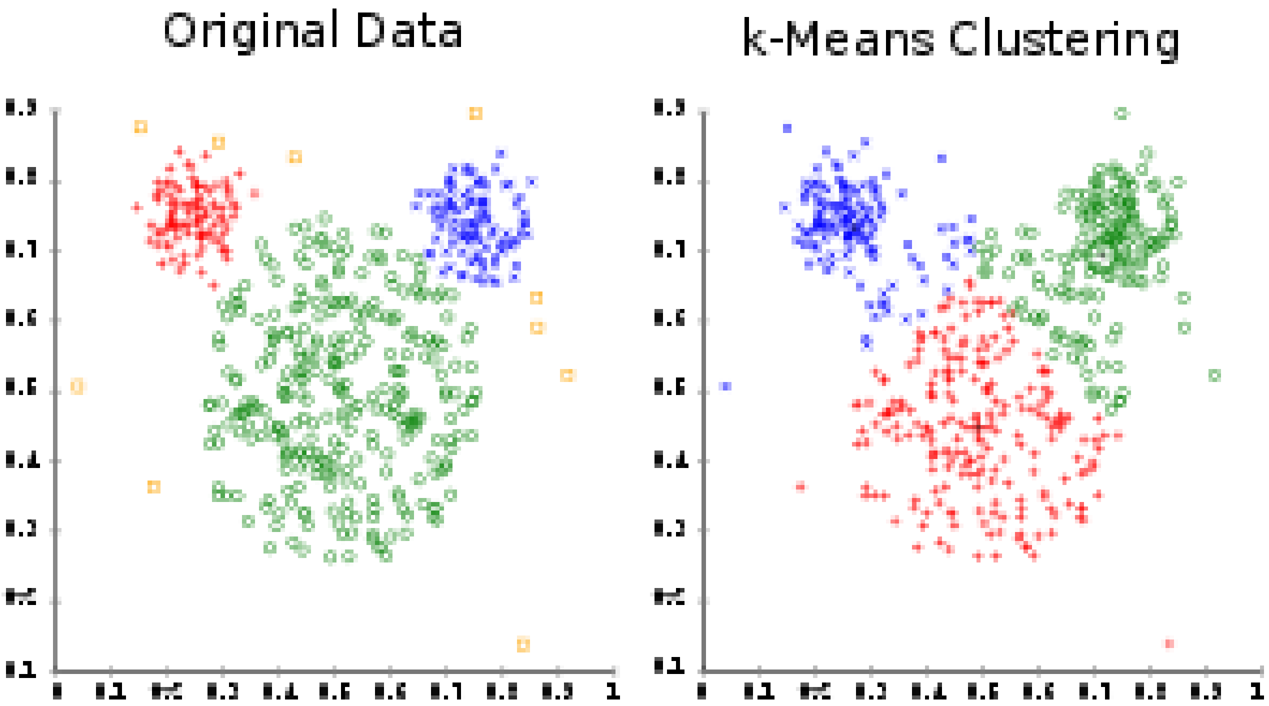
- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
    - Local optima



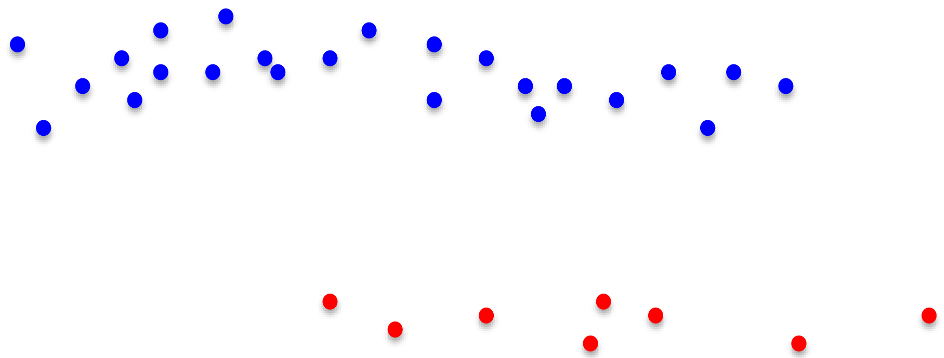




Inductive Bias



Equally Sized Clusters



Circular Clusters

Summary

- Clustering
  - Group together similar instances
- K-means
  - Assign data instances to closest mean
  - Assign each mean to the average of its assigned points