

# Announcement

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- Proposal presentation on Dec. 14 & 16
- Problem set 5 is out, due Dec 9
- Homework 5 is out

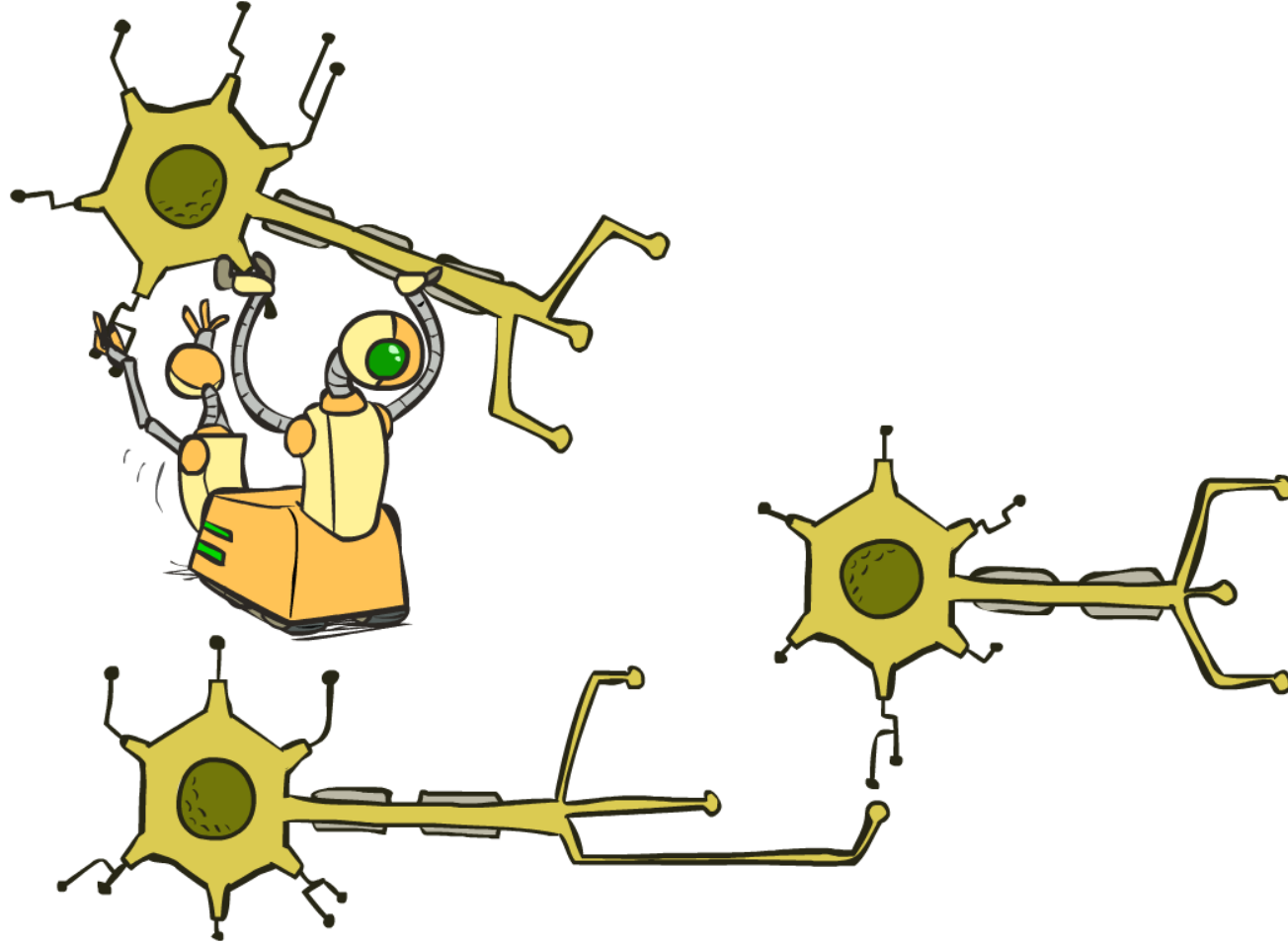
# Proposal Presentation

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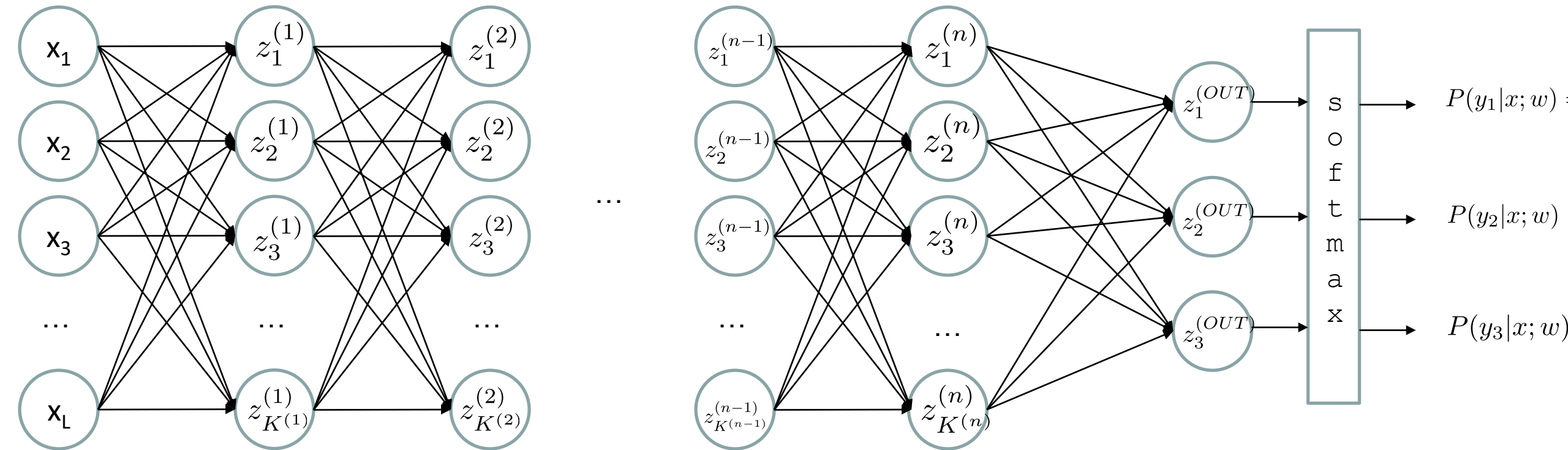
- Proposal presentation
  - 4-5 min presentation: topic, motivation, possible methods
  - Dec. 14, 16, in class
  - Presentation schedule will be sent out later
- If you have not formed/joined a group, please do so ASAP
  - Group registration: <https://wj.qq.com/s2/7551413/2fd0/>

# Neural Networks

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# Deep Neural Network = Also learn the features!

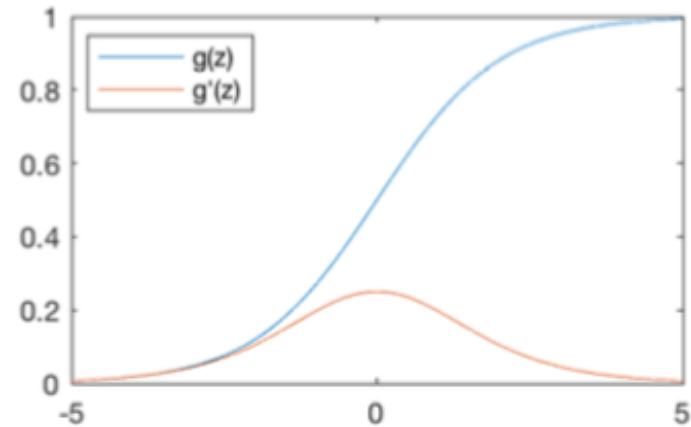


$$z_i^{(k)} = g\left(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)}\right)$$

**g = nonlinear activation function**

# Common Activation Functions

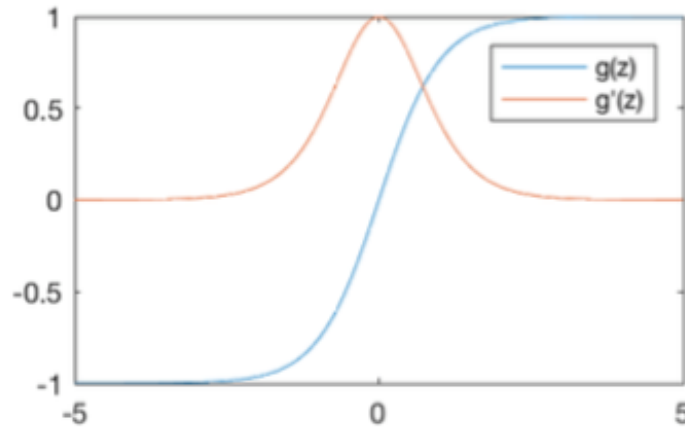
Sigmoid Function



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

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

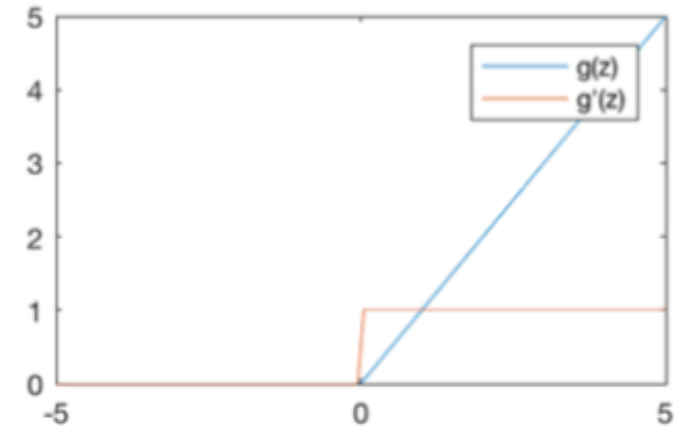
Hyperbolic Tangent



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

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

Rectified Linear Unit (ReLU)



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

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

# Deep Neural Network: Also Learn the Features!

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

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

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

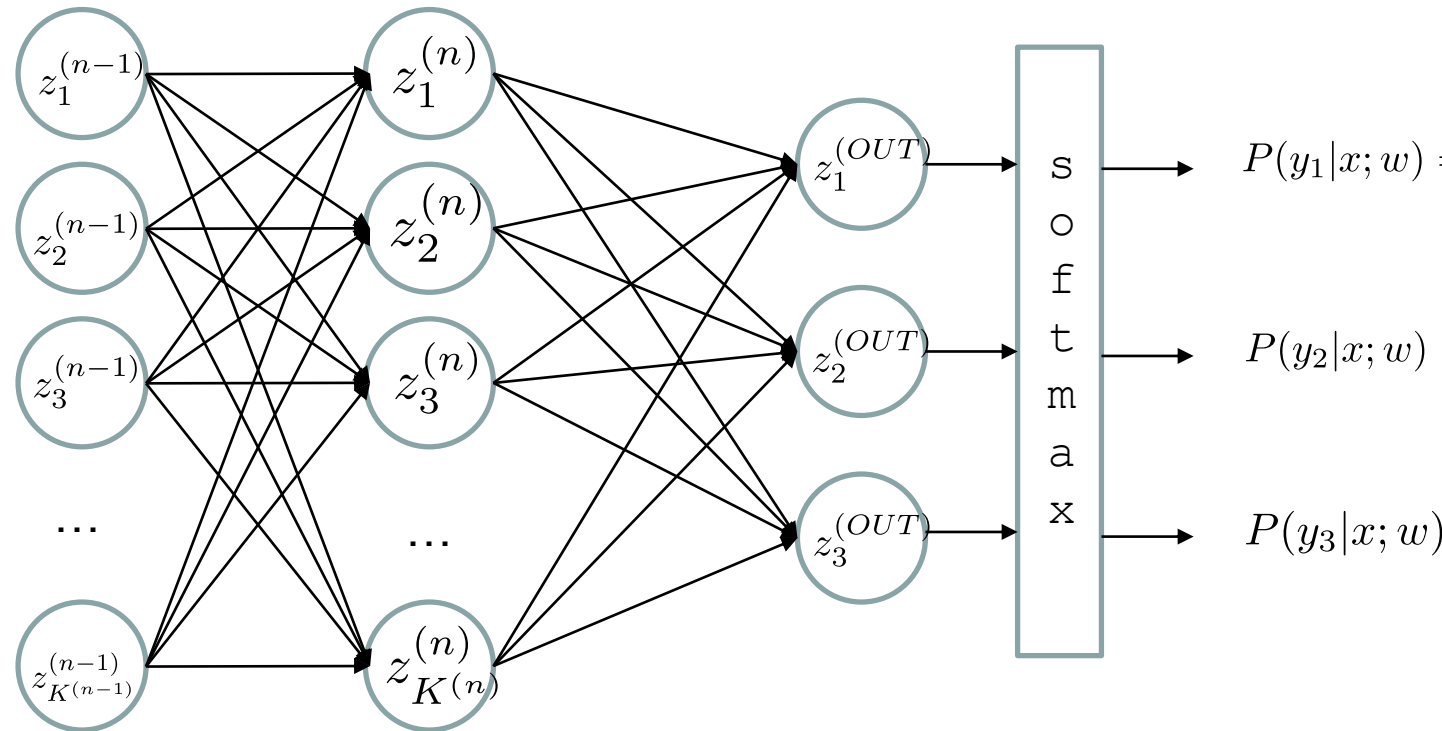
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- Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.
- Practical considerations
  - Can be seen as learning the features
  - Large number of neurons
    - Danger for overfitting
    - (hence early stopping!)

# Training a Network

## Key words:

- Forward
- Backwards
- Gradient
- Backprop



**g = nonlinear activation function**

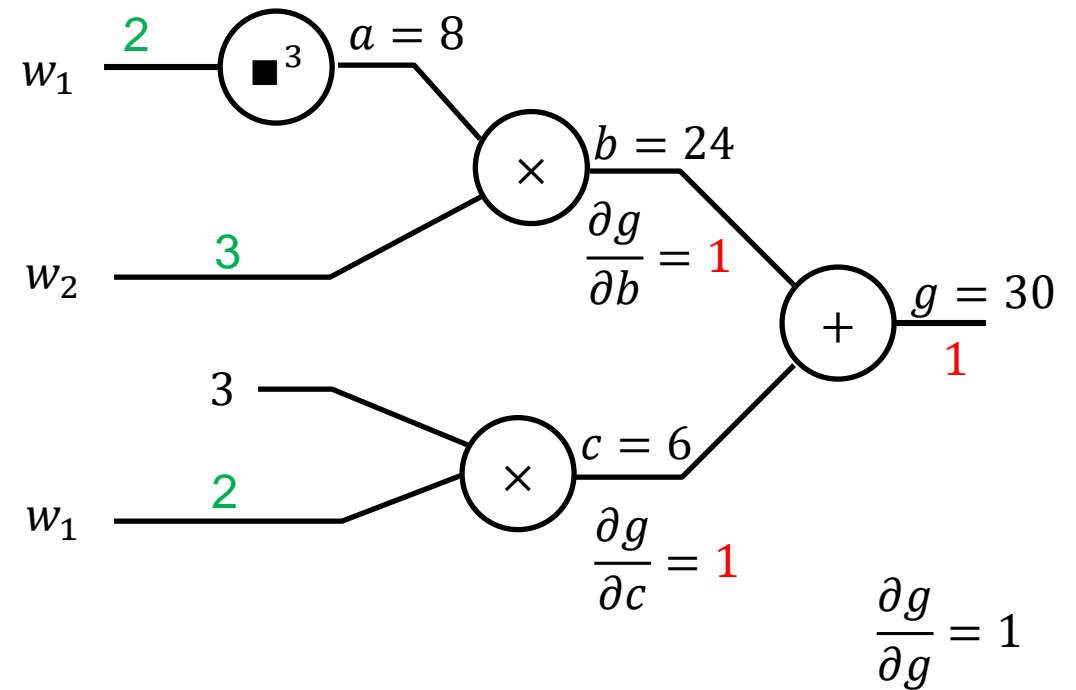


# Back Propagation: $g(\mathbf{w}) = w_1^3 w_2 + 3w_1$

- Suppose we have  $g(\mathbf{w}) = w_1^3 w_2 + 3w_1$  and want the gradient at  $\mathbf{w} = [2, 3]$
- 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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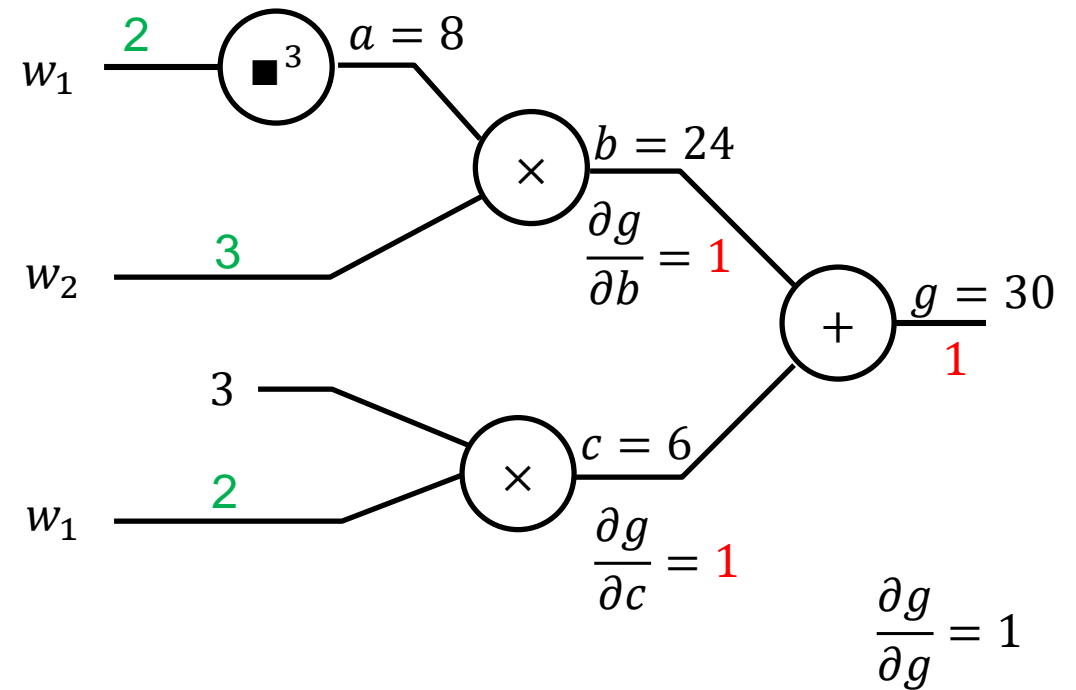
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- $\frac{\partial g}{\partial a} = \frac{\partial g}{\partial b} \frac{\partial b}{\partial a}$



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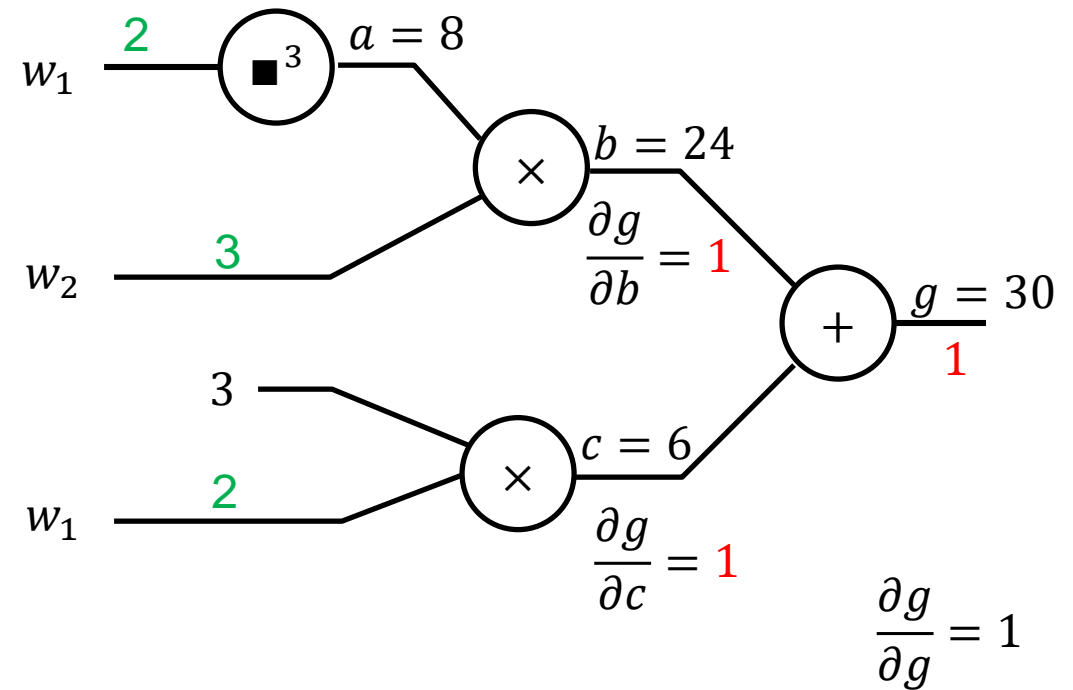
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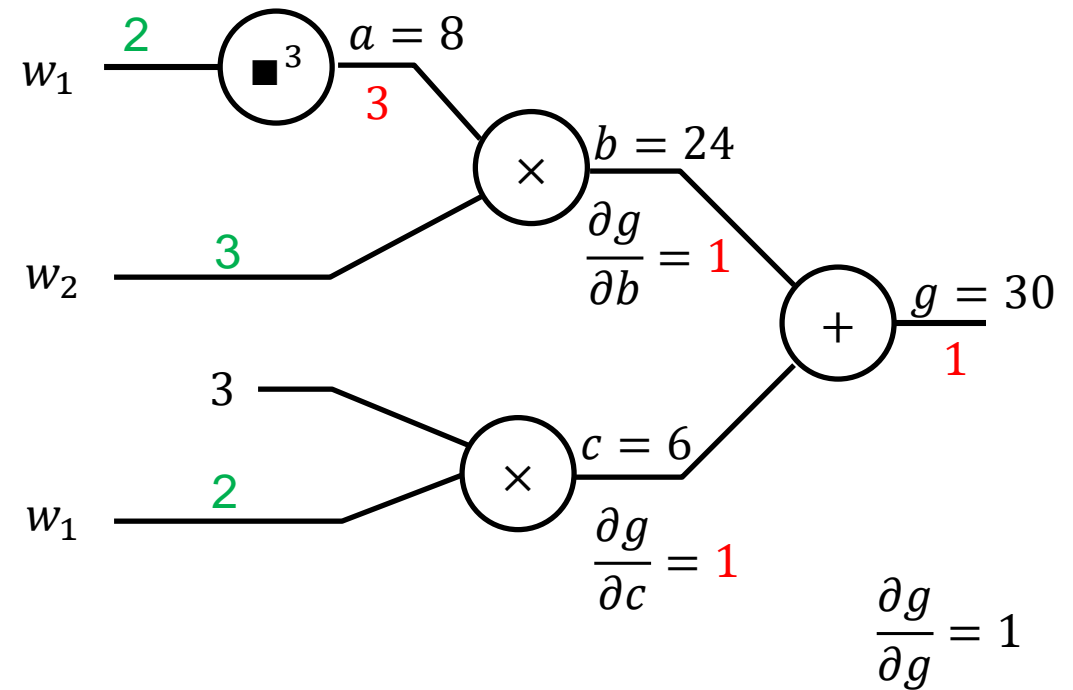
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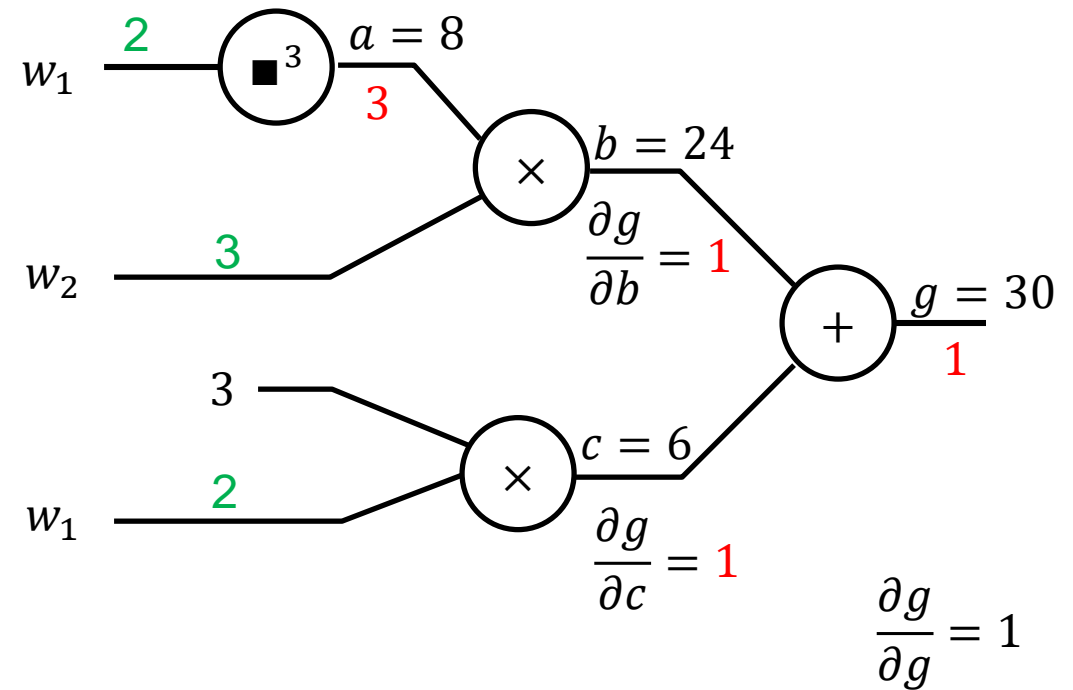
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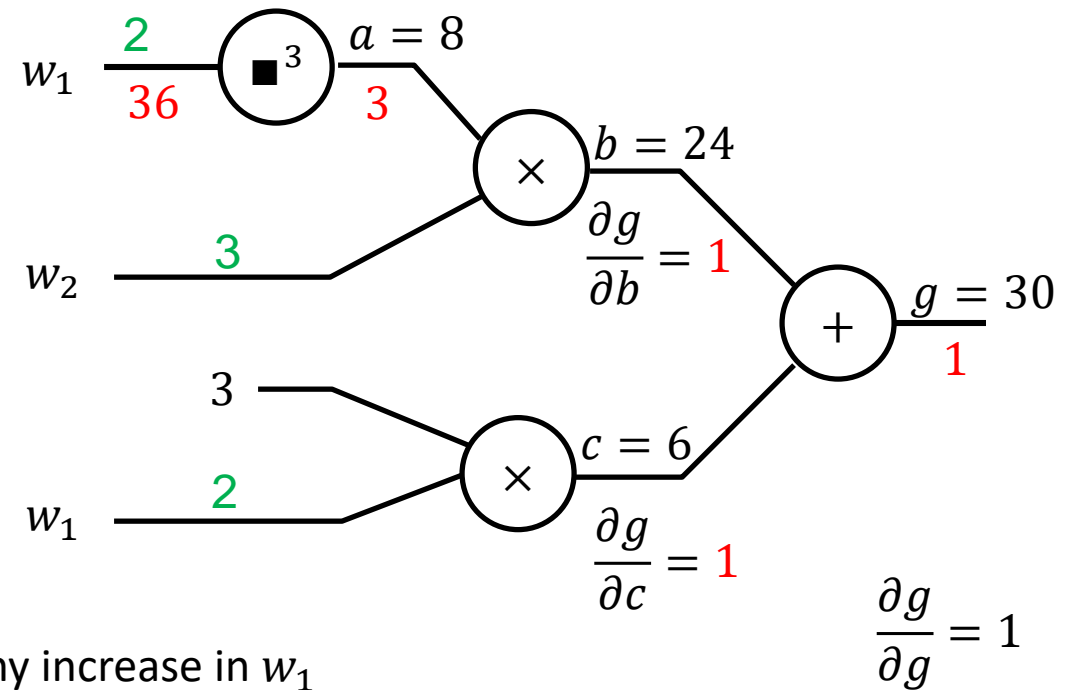
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- $\frac{\partial g}{\partial w_1} = \frac{\partial g}{\partial a} \frac{\partial a}{\partial w_1} = 3 \cdot 3w_1^2 = 36$



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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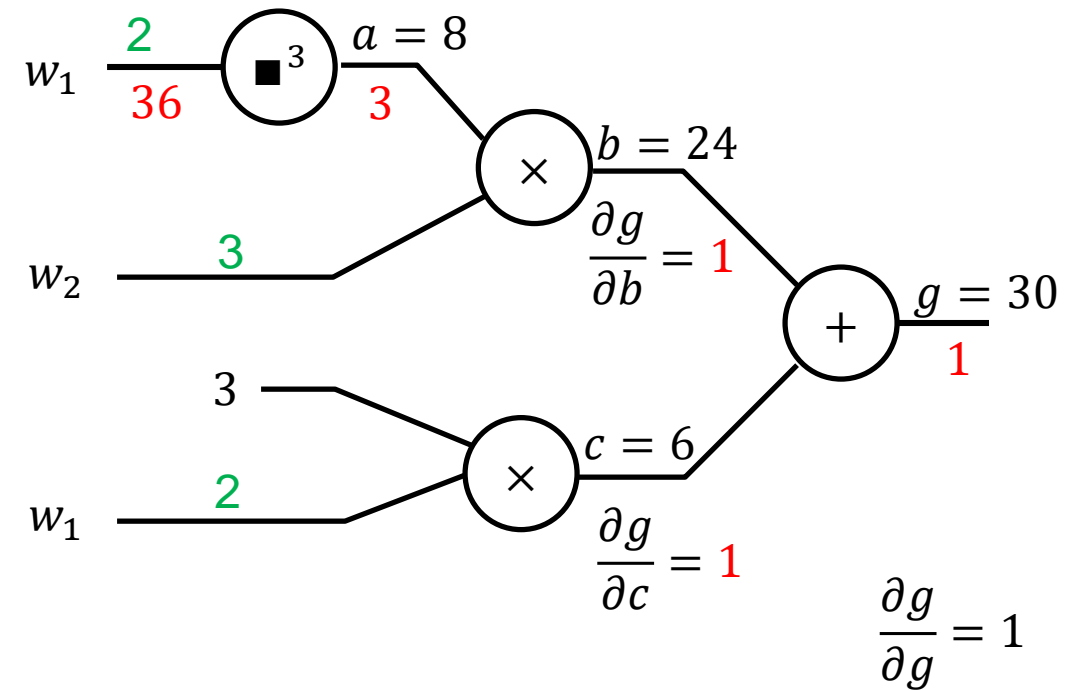
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- $\frac{\partial g}{\partial w_2} = ???$  Hint:  $b = a \times 3$  may be useful.



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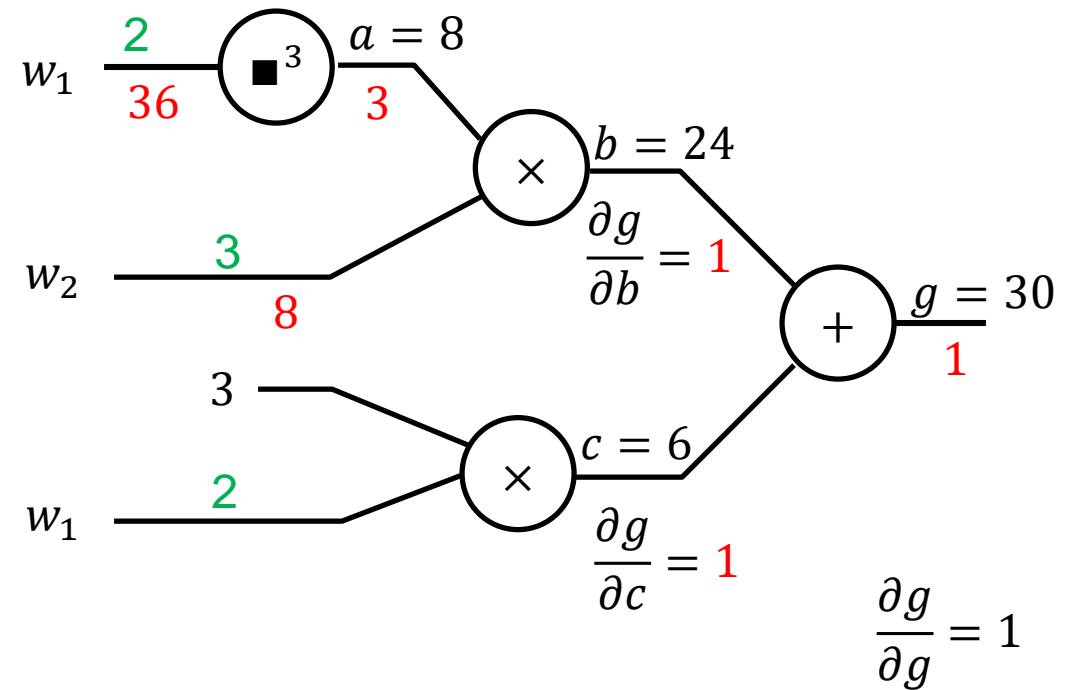
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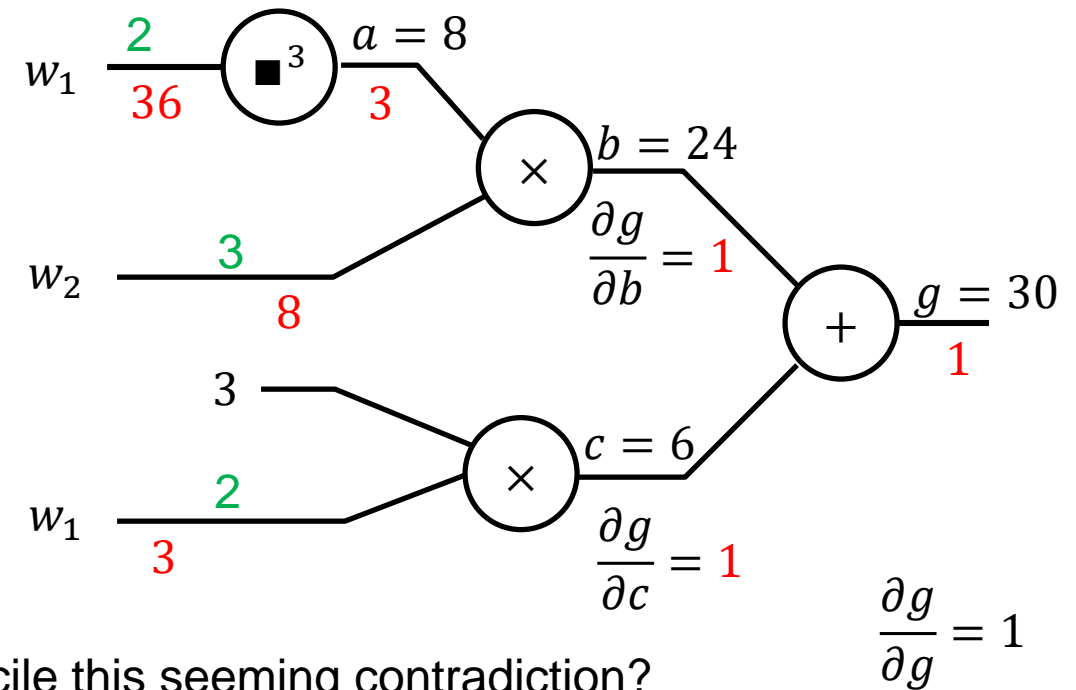
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How do we reconcile this seeming contradiction?  
Top partial derivative means cube function contributes  $36w_1$  and bottom p.d. means product contributes  $3w_1$  so add them.

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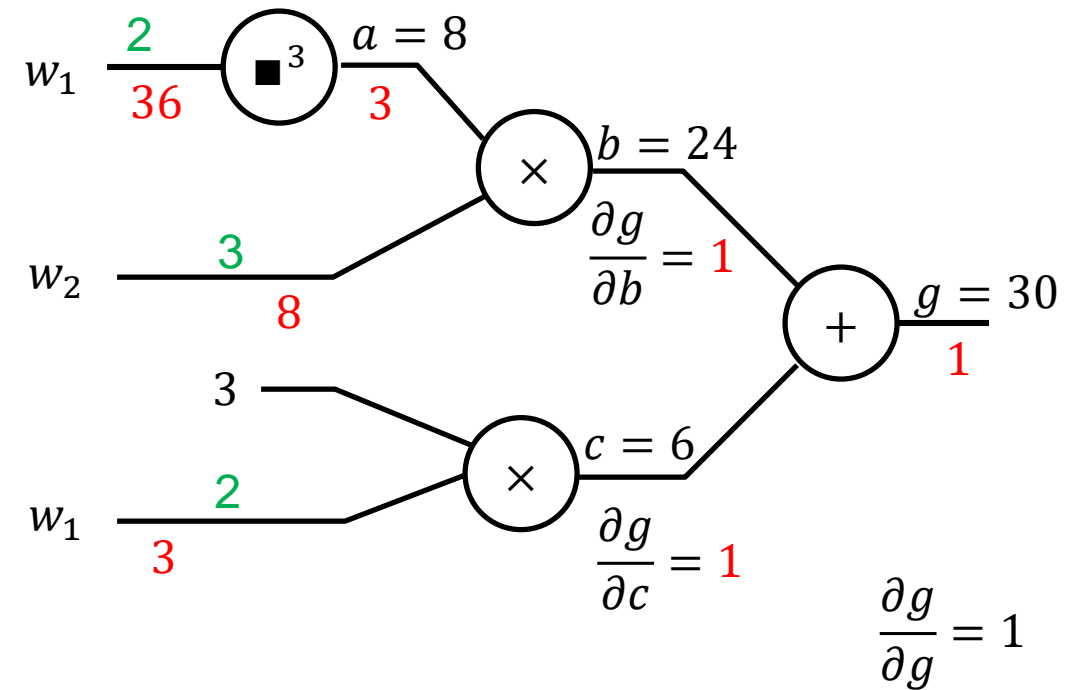
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$$\nabla g = \left[ \frac{\partial g}{\partial w_1}, \frac{\partial g}{\partial w_2} \right] = [39, 8]$$

# 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:  $O(NM)$

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

# Automatic Differentiation

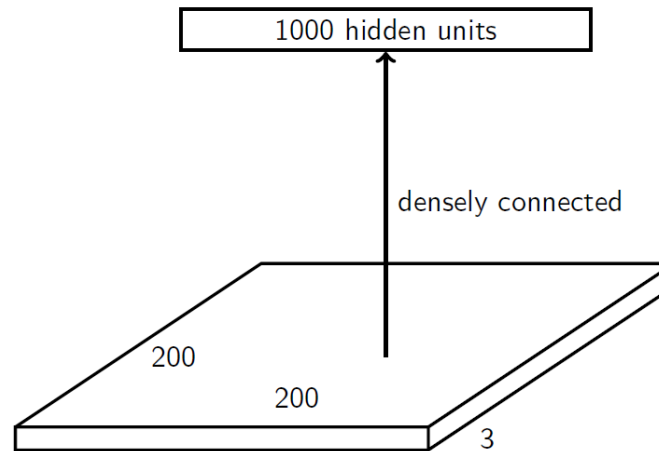
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- Automatic differentiation software
  - e.g. Theano, TensorFlow, PyTorch, Chainer
  - Only need to program the function  $g(x,y,w)$
  - Can automatically compute all derivatives w.r.t. all entries in  $w$
  - This is typically done by caching info 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

# Convolutional Neural Networks

- Visual recognition

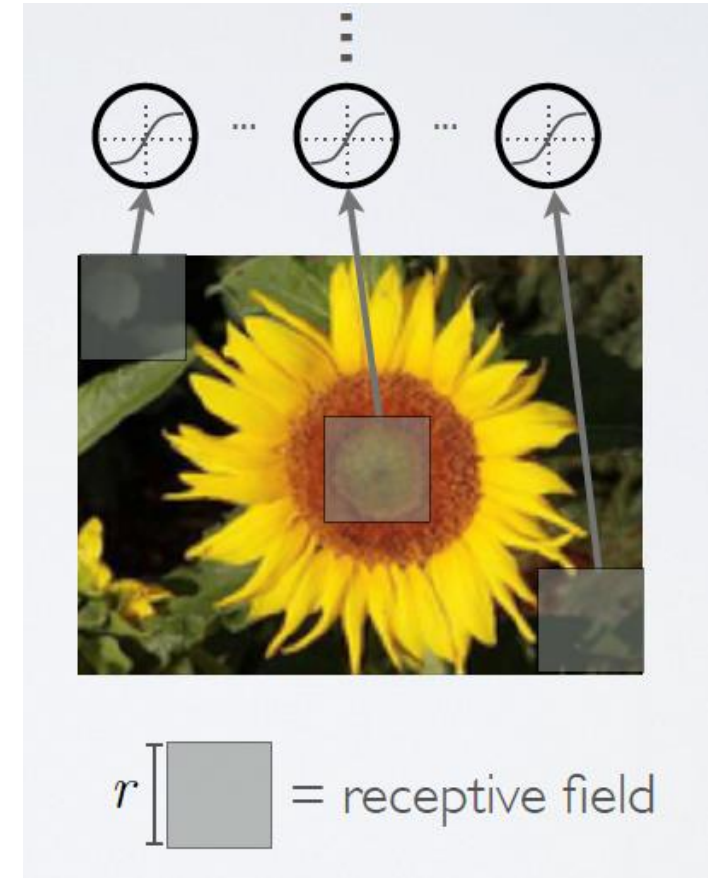
- Suppose we aim to train a network that takes a 200x200 RGB image as input



- What is the problem with have full connections in the first layer?
  - Too many parameters!  $200 \times 200 \times 3 \times 1000 = 120$  million
  - What happens if the object in the image shifts a little?

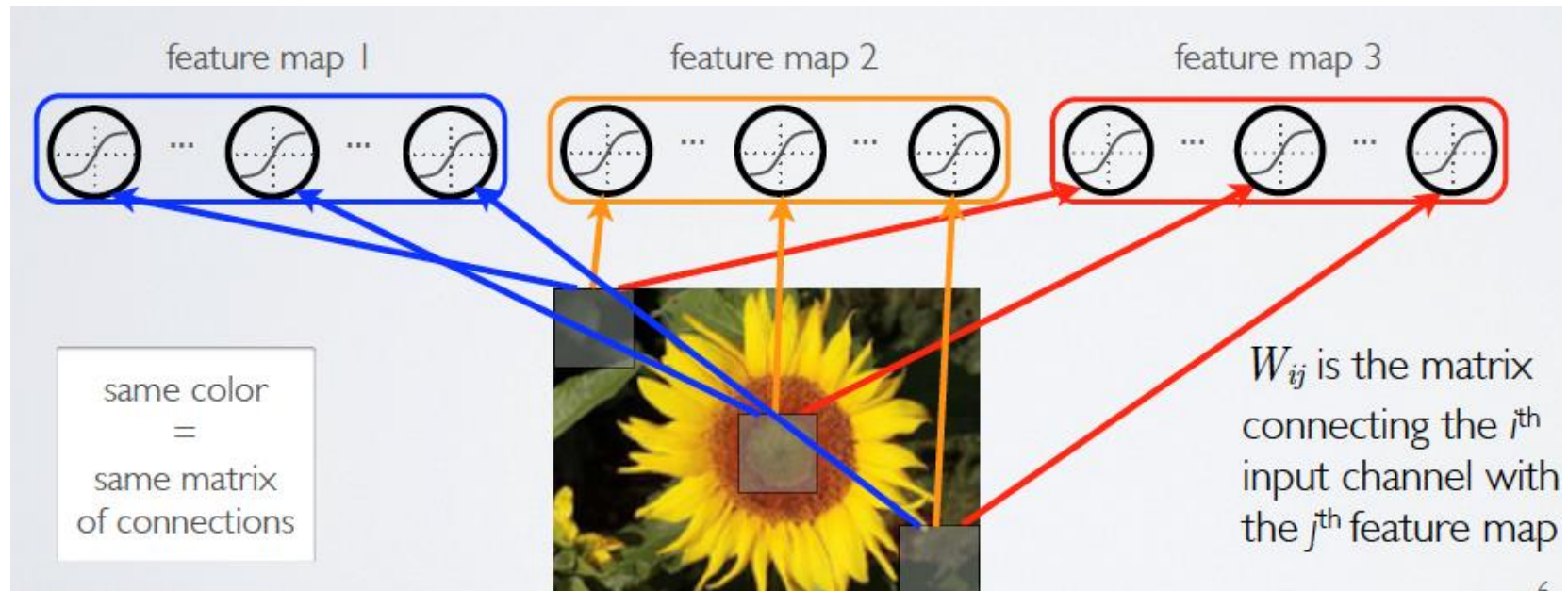
# Overview of CNNs

- First idea: Use a local connectivity of hidden units
  - Each hidden unit is connected only to a subregion (patch) of the input image
  - Usually it is connected to all channels
  - Each neuron has a local receptive field



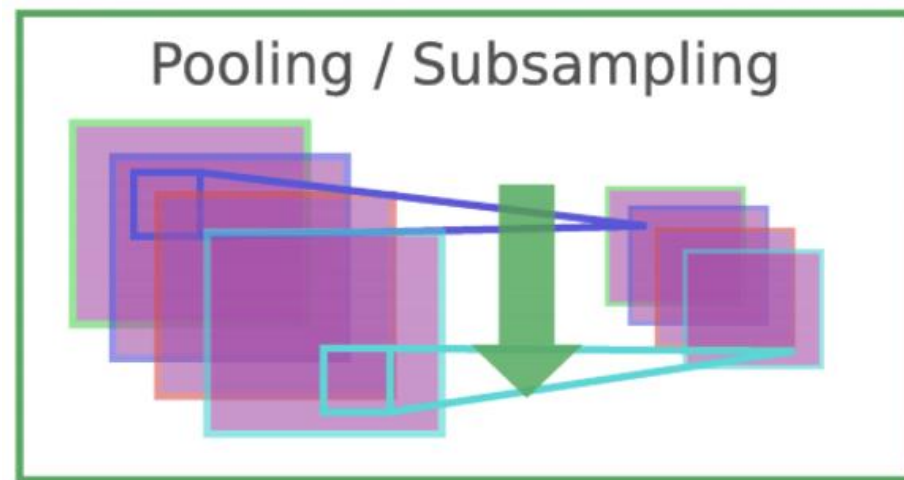
# Overview of CNNs

- Second idea: share weights across certain units
  - Units organized into the same “feature map” share weight parameters
  - Hidden units within a feature map cover different positions in the image



# Overview of CNNs

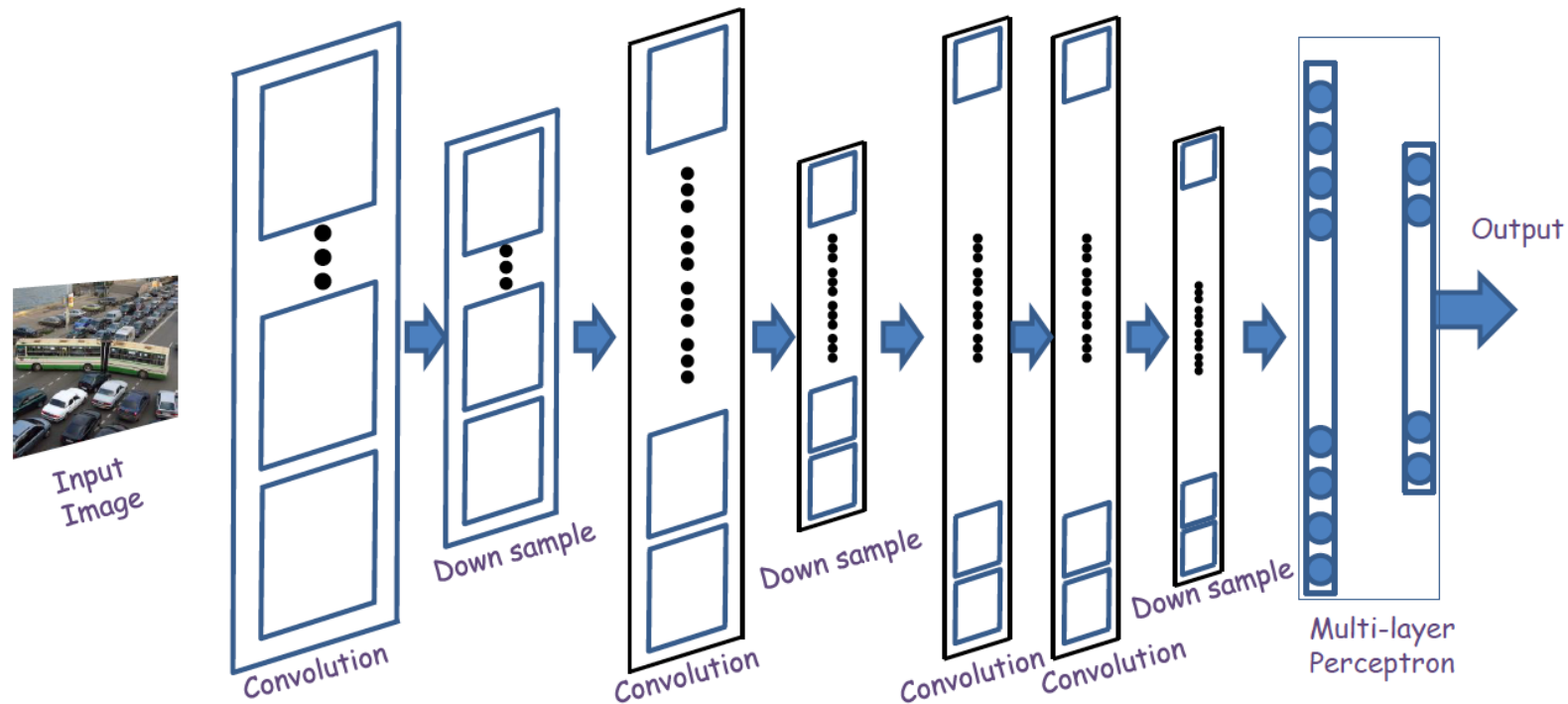
- Third idea: pool hidden units in the same neighborhood
  - Averaging or Discarding location information in a small region
  - Robust toward small deformations in object shapes by ignoring details.





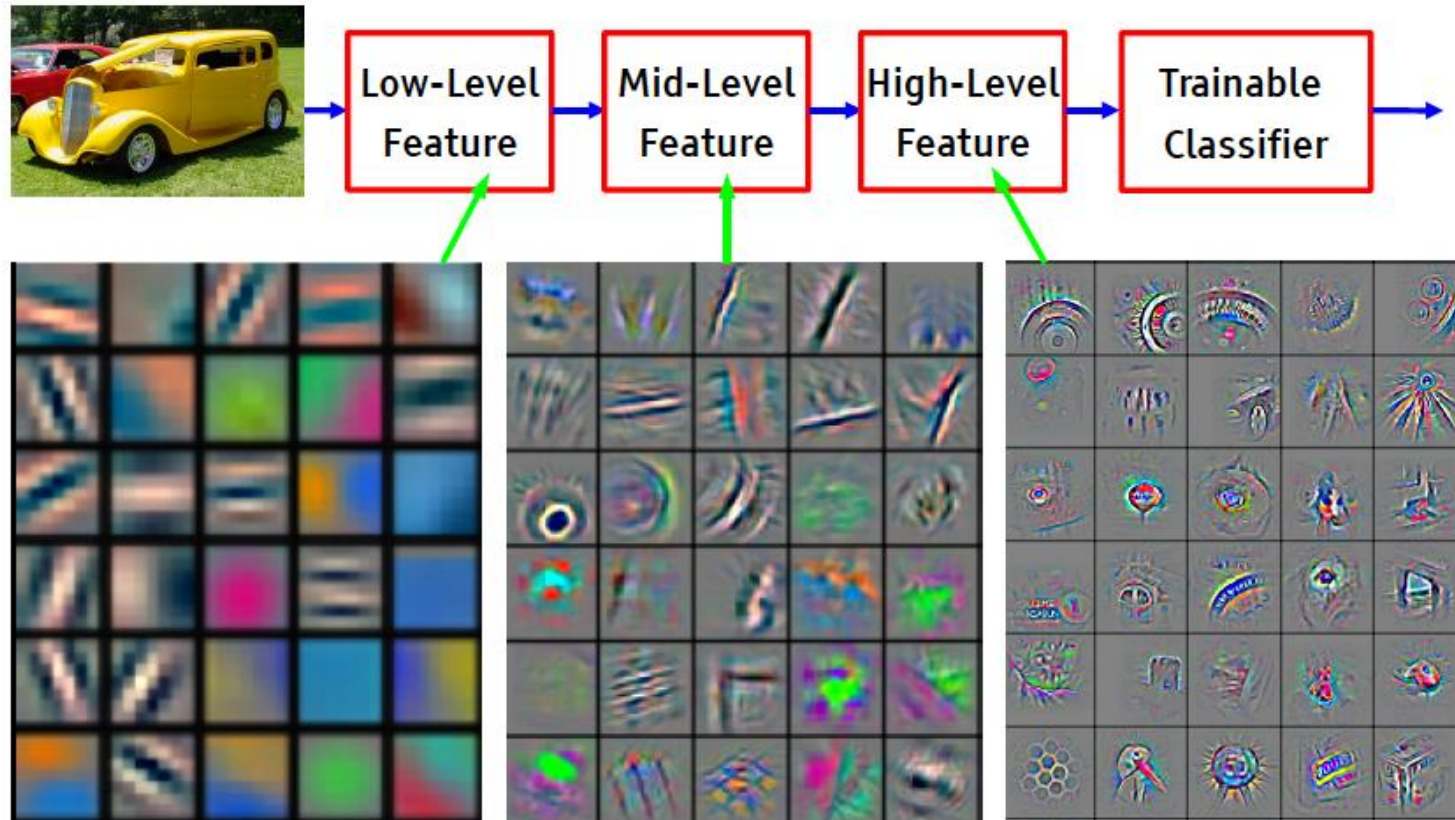
# Overview of CNNs

- Fourth idea: Interleaving feature extraction and pooling operations
  - Extracting abstract, compositional features for representing semantic object classes



# Overview of CNNs

- Artificial visual pathway: from images to semantic concepts (Representation learning)



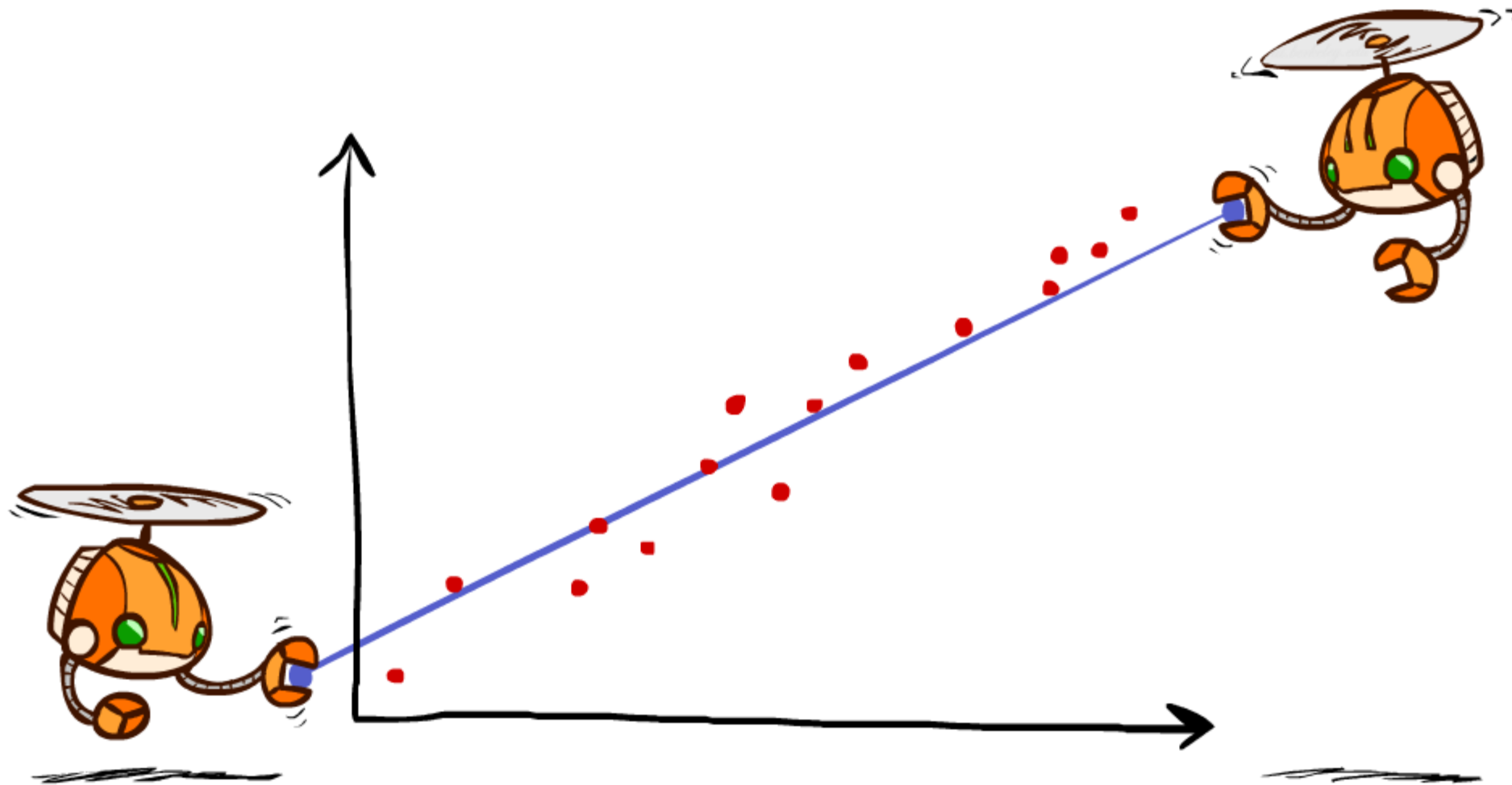
Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

# More classification methods

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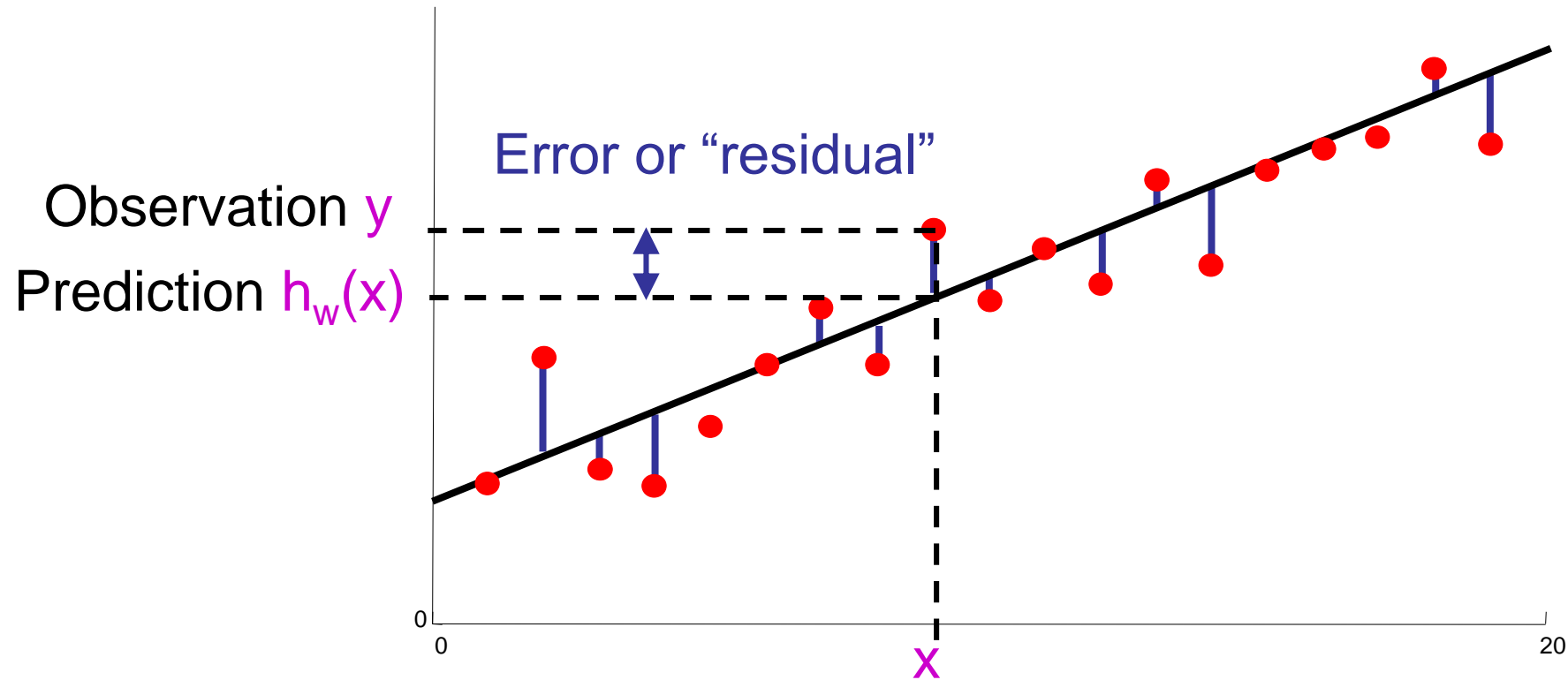
- Naive Bayes
- Perceptron / Neural networks
- Decision trees / Random forest
- Support Vector Machines
- Nearest neighbors
- Model ensembles: bagging, boosting, etc.
- .....

# Regression



# Linear Regression

Prediction:  $h_w(x) = w_0 + w_1x$



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

# Least squares: Minimizing squared error

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

$$L(\mathbf{w}) = \sum_i (y_i - h_{\mathbf{w}}(\mathbf{x}_i))^2 = \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

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

# Regularized Regression

- Overfitting is also possible in regression
  - Extreme case:  $n$  features,  $n$  training examples
- Regularization can be used to alleviate overfitting
- LASSO (Least Absolute Shrinkage and Selection Operator)

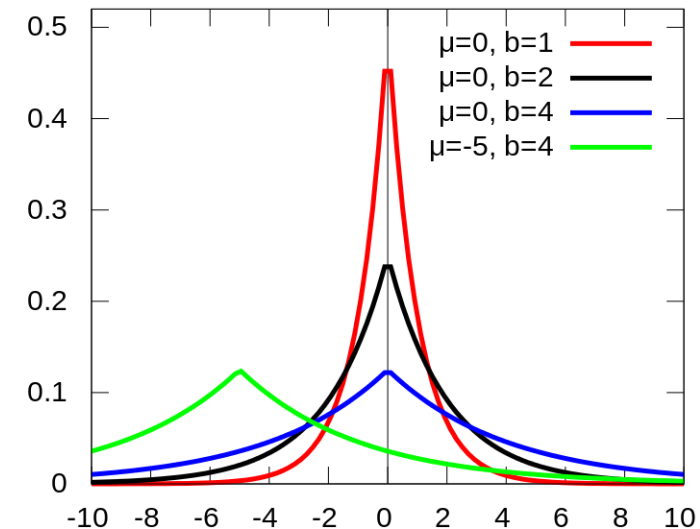
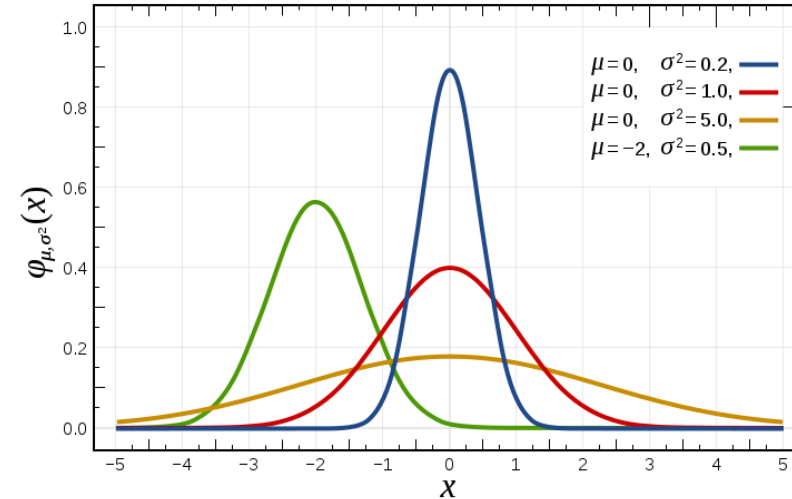
$$L(\mathbf{w}) = \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \lambda \sum_k |w_k|$$

- Ridge Regression

$$L(\mathbf{w}) = \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \lambda \sum_k w_k^2$$

# Regularized Regression

- L2 regularization = Gaussian distribution as weight prior
  - Small weights
- L1 regularization = Laplace distribution as weight prior
  - Long-tailed distribution
  - Zero weights + sparse large weights





# Non-linear least squares

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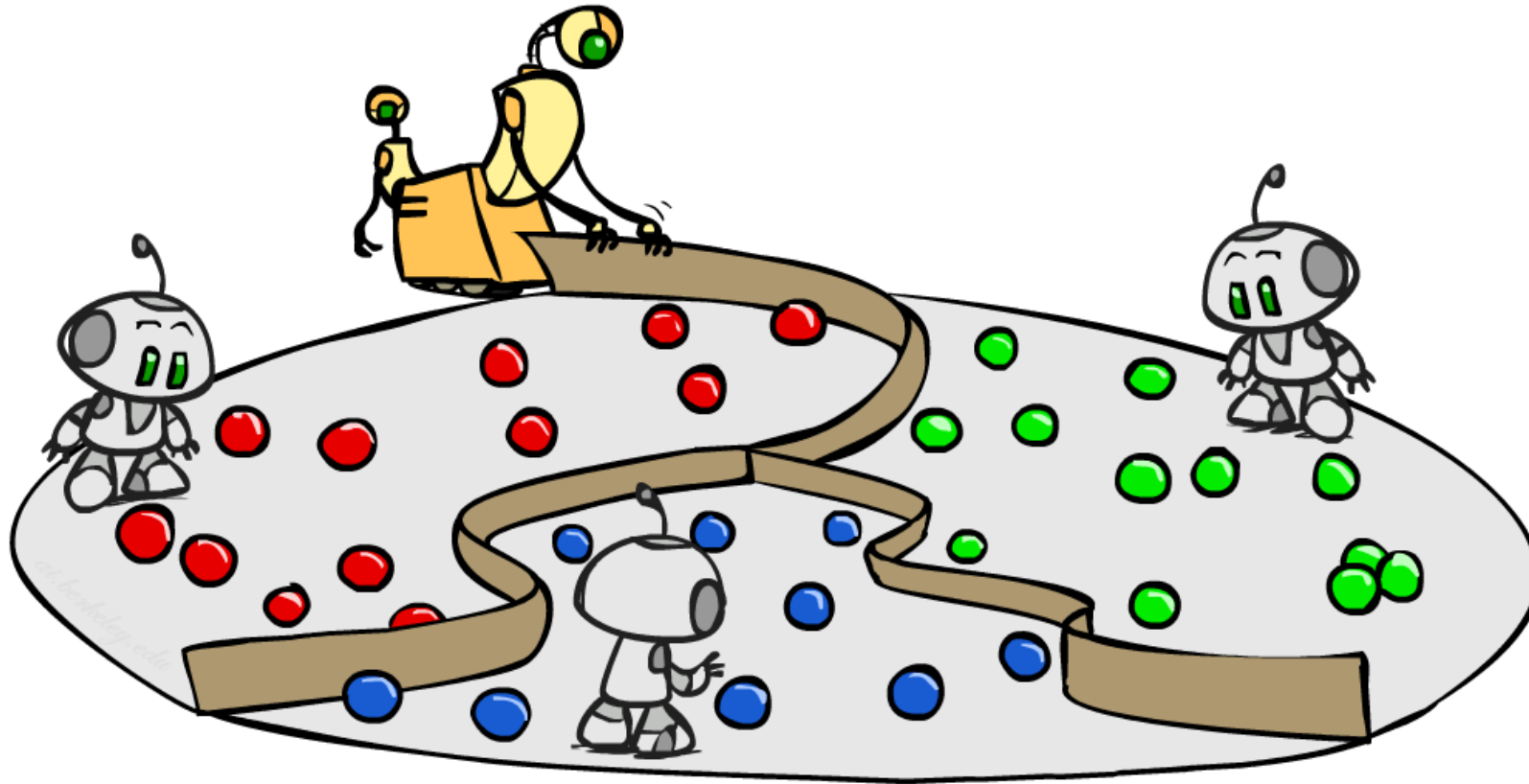
- No closed-form solution in general
- Numerical algorithms are typically used
  - Choose initial values for the parameters and then refine the parameters iteratively
  - Gradient descent
  - Gauss–Newton method
  - Limited-memory BFGS
  - Derivative-free methods
  - etc.

# Summary

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- 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

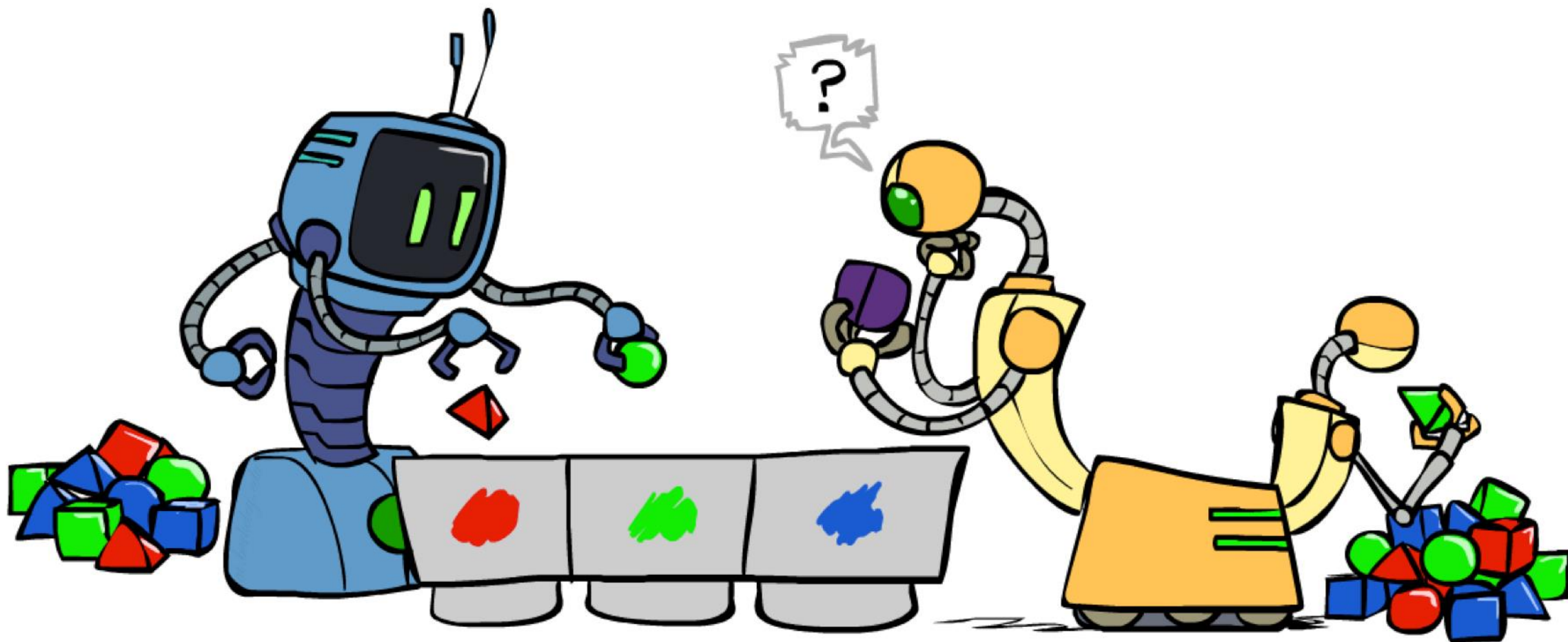
[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley and from Daniel Weld, Carlos Guestrin, & Luke Zettlemoyer at U Washington]

# Types of Learning

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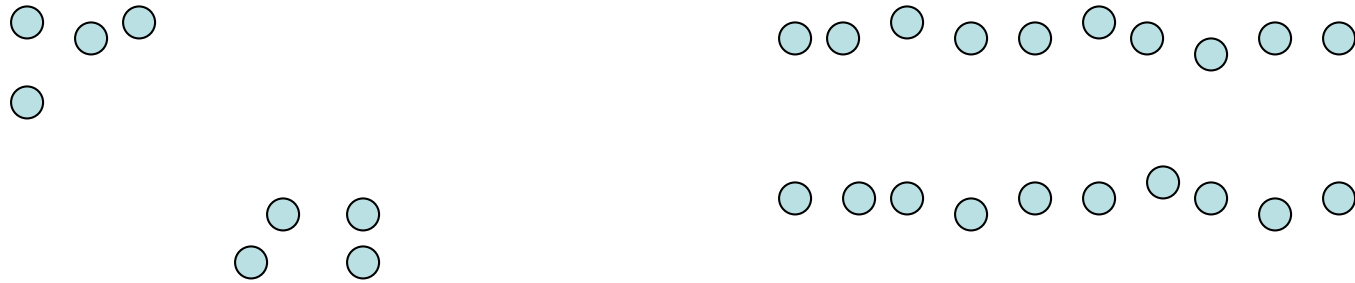
- Supervised learning
  - Training data includes desired outputs
- Unsupervised learning 
  - Training data does not include desired outputs
- Semi-supervised learning
  - Training data includes a few desired outputs
- Reinforcement learning
  - Rewards from sequence of actions

# 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



**World »** [edit](#)

**[Heavy Fighting Continues As Pakistan Army Battles Taliban](#)**  
Voice of America - 10 hours ago  
By Barry Newhouse Pakistan's military said its forces have killed 55 to 60 Taliban militants in the last 24 hours in heavy fighting in Taliban-held areas of the northwest.  
[Pakistani troops battle Taliban militants for fourth day](#) guardian.co.uk  
[Army: 55 militants killed in Pakistan fighting](#) The Associated Press  
[Christian Science Monitor](#) - [CNN International](#) - [Bloomberg](#) - [New York Times](#)  
[all 3,824 news articles »](#)

**[Sri Lanka admits bombing safe haven](#)**  
guardian.co.uk - 3 hours ago  
Sri Lanka has admitted bombing a "safe haven" created for up to 150000 civilians fleeing fighting between Tamil Tiger fighters and the army.  
[Chinese billions in Sri Lanka fund battle against Tamil Tigers](#) Times Online  
[Huge Humanitarian Operation Under Way in Sri Lanka](#) Voice of America  
[BBC News](#) - [Reuters](#) - [AFP](#) - [Xinhua](#)  
[all 2,492 news articles »](#)

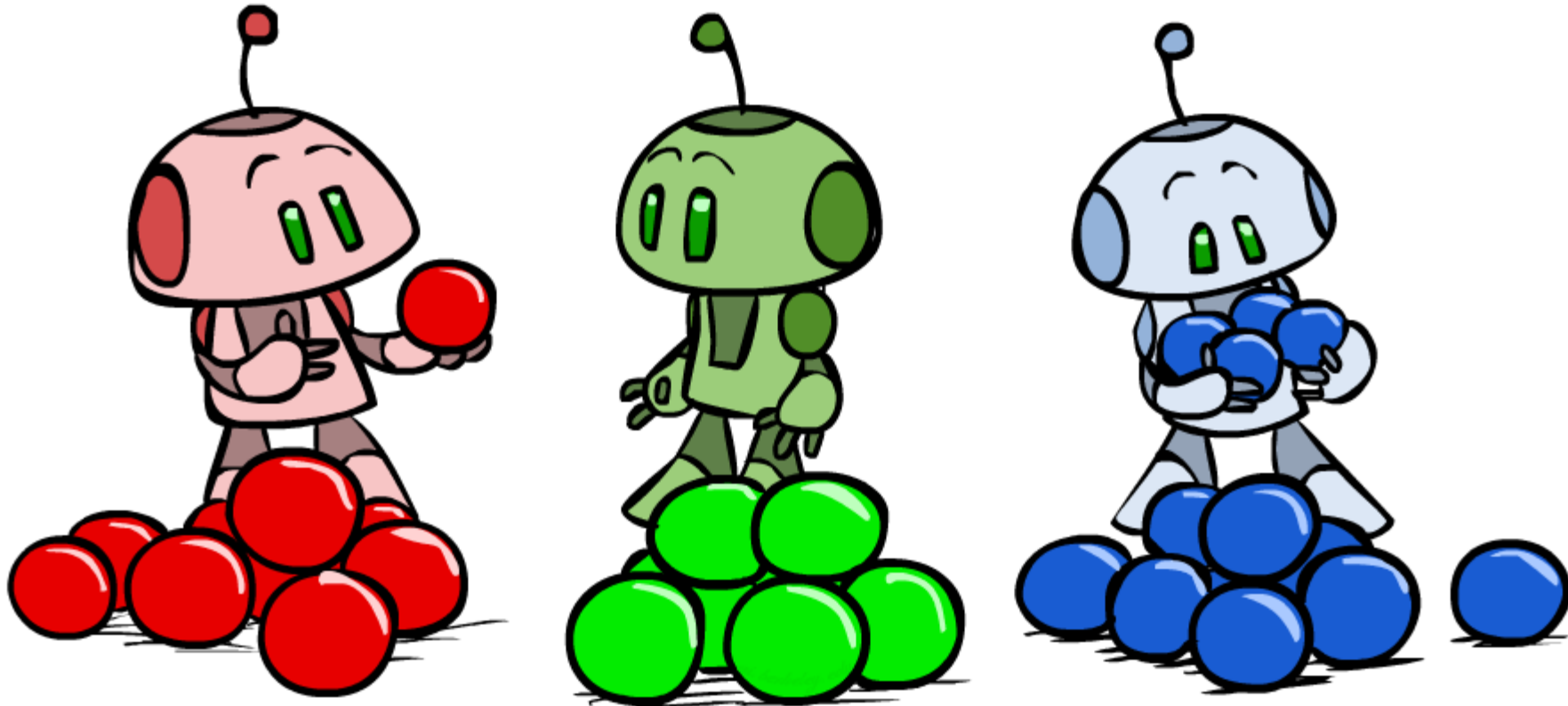
**Business »** [edit](#)

**[Buffett Calls Investment Candidates' 2008 Performance Subpar](#)**  
Bloomberg - 2 hours ago  
By Hugh Son, Erik Holm and Andrew Frye May 2 (Bloomberg) -- Billionaire Warren Buffett said all of the candidates to replace him as chief investment officer of Berkshire Hathaway Inc. failed to beat the 38 percent decline of the Standard & Poor's 500 ...  
[Buffett offers bleak outlook for US newspapers](#) Reuters  
[Buffett Limit CEO pay through embarrassment](#) MarketWatch  
[CNBC](#) - [The Associated Press](#) - [guardian.co.uk](#)  
[all 1,454 news articles »](#)

**[Chrysler's Fall May Help Administration Reshape GM](#)**  
New York Times - 5 hours ago  
Auto task force members, from left: Treasury's Ron Bloom and Gene Sperling, Labor's Edward Montgomery, and Steve Rattner. BY DAVID E. SANGER and BILL VLASIC  
WASHINGTON - Fresh from pushing Chrysler into bankruptcy, President Obama and his economic team ...  
[Comment by Gary Chaison](#) Prof. of Industrial Relations, Clark University  
[Bankruptcy reality sets in for Chrysler, workers](#) Detroit Free Press  
[Washington Post](#) - [Bloomberg](#) - [CNNMoney.com](#)  
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# K-Means

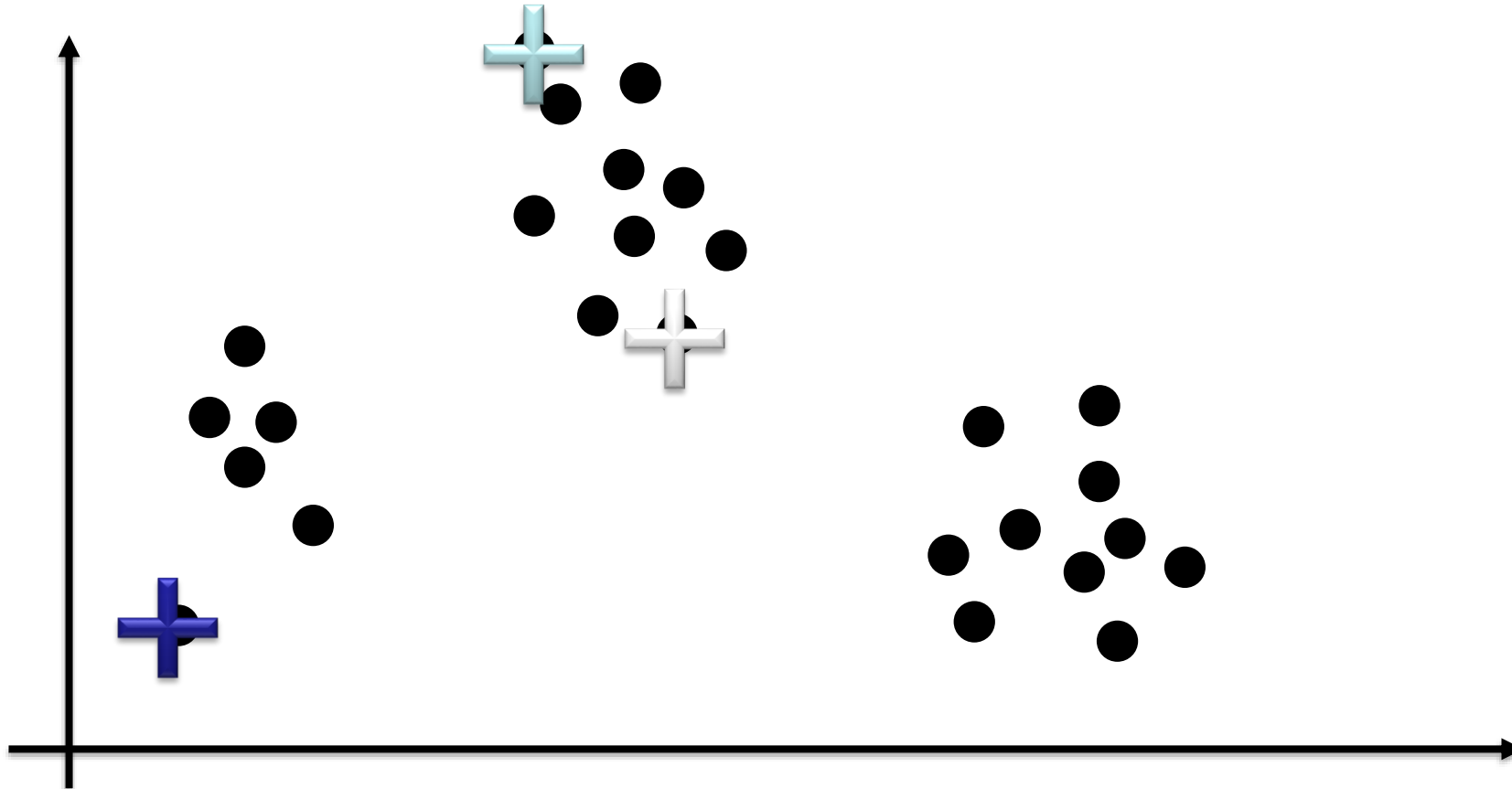
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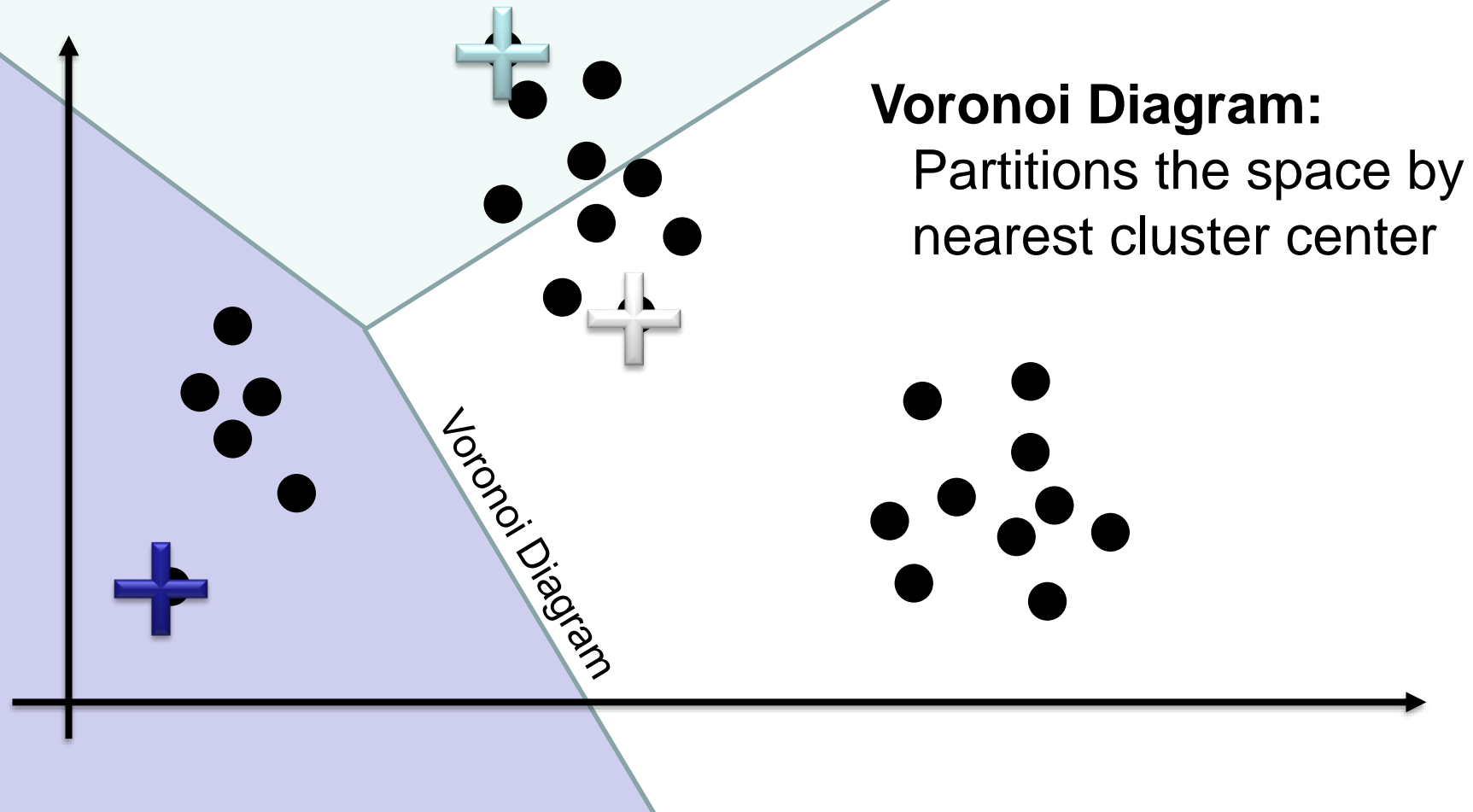
# K-Means Clustering: *Intuition*

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



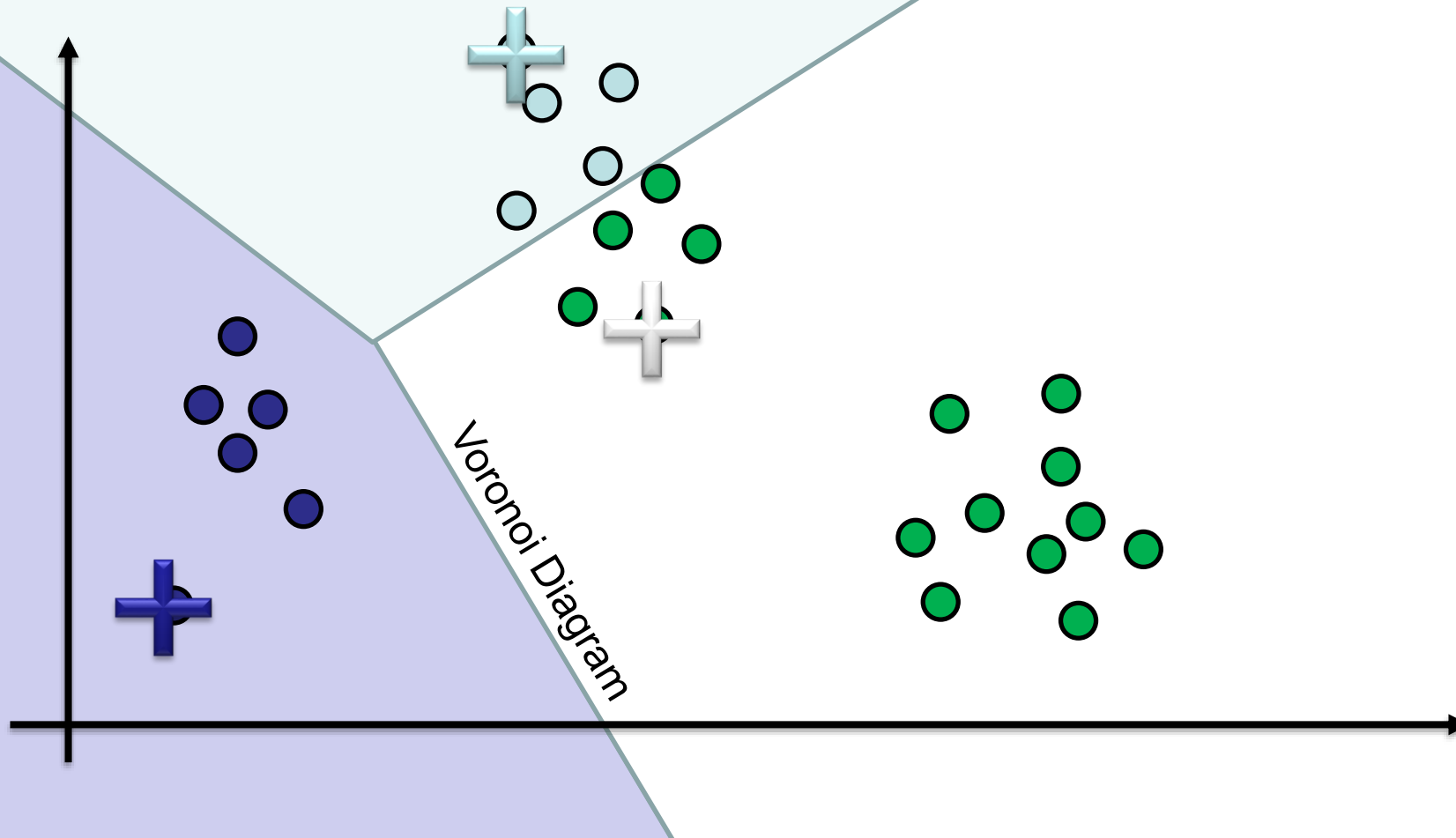
# K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



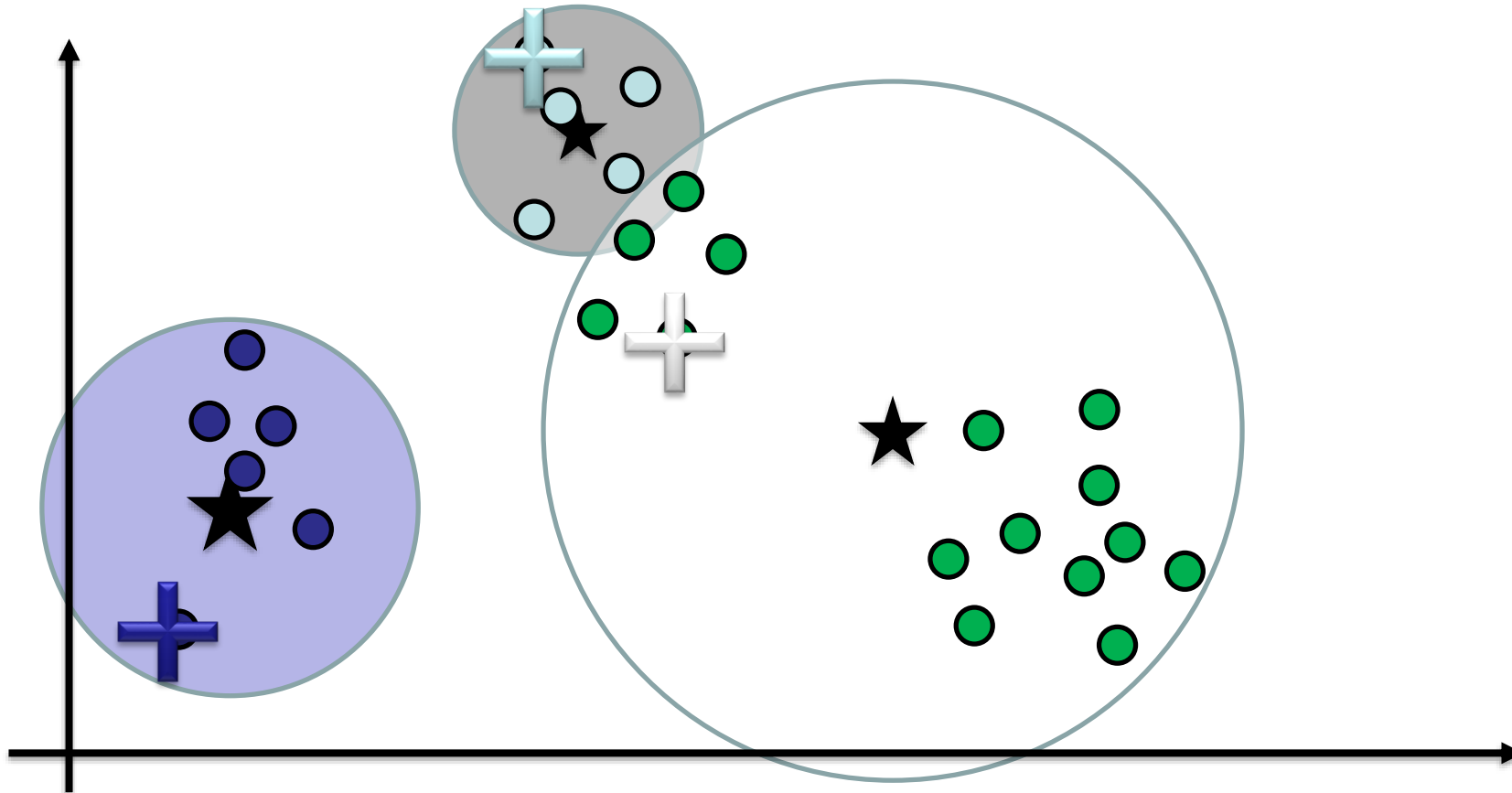
# K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



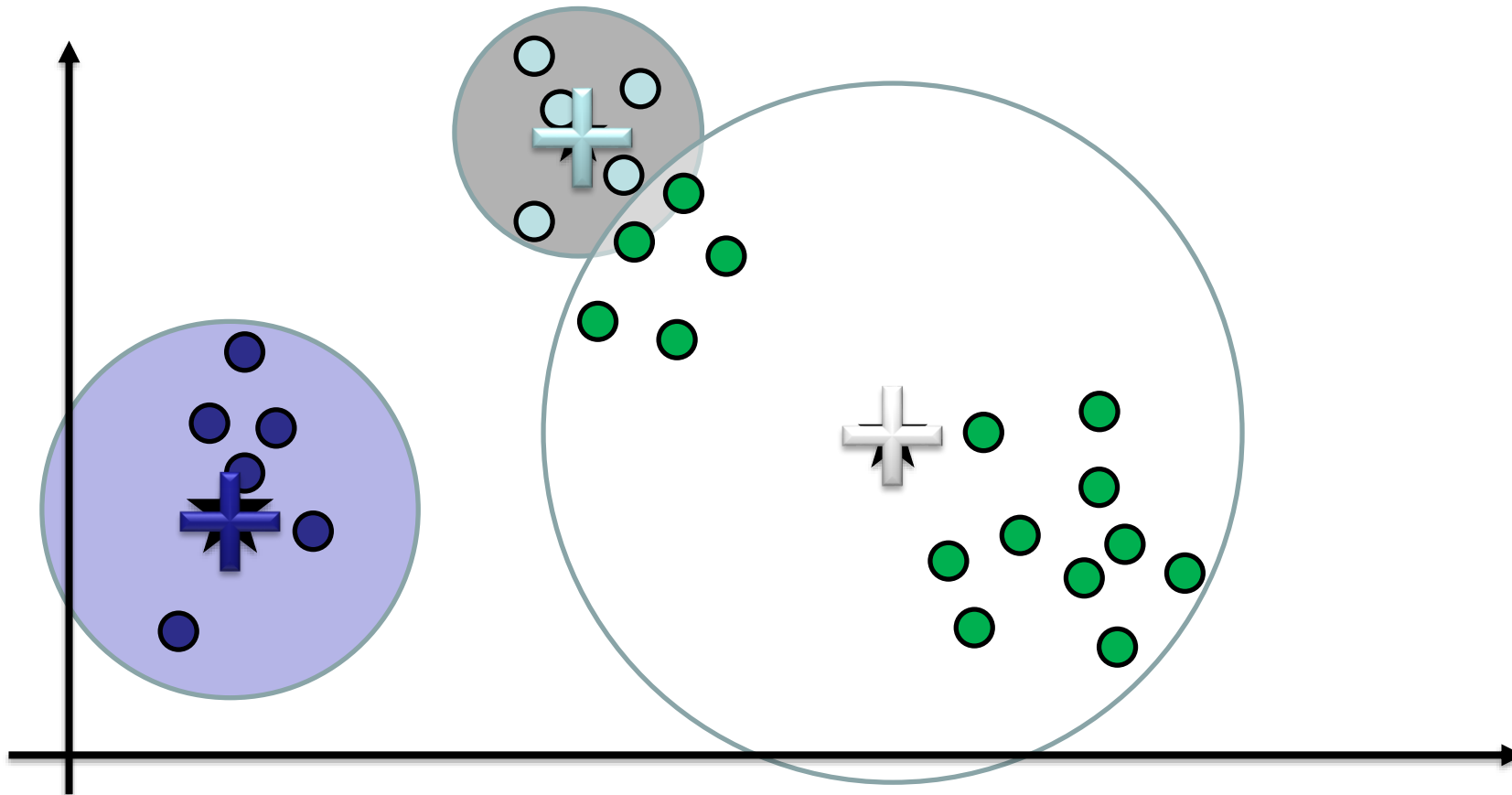
# K-Means Clustering: *Intuition*

- Compute mean of points in each “cluster”



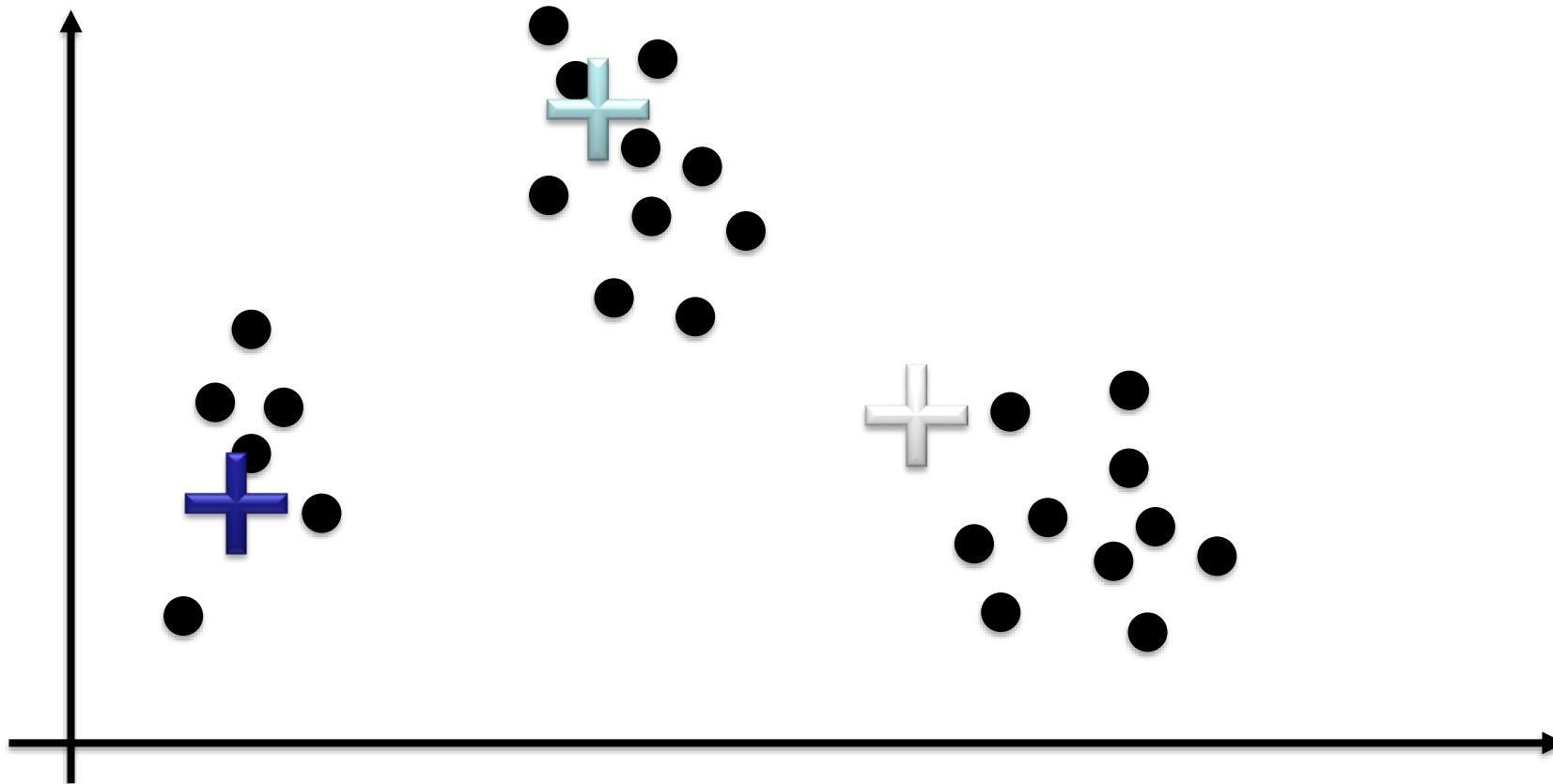
# K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster



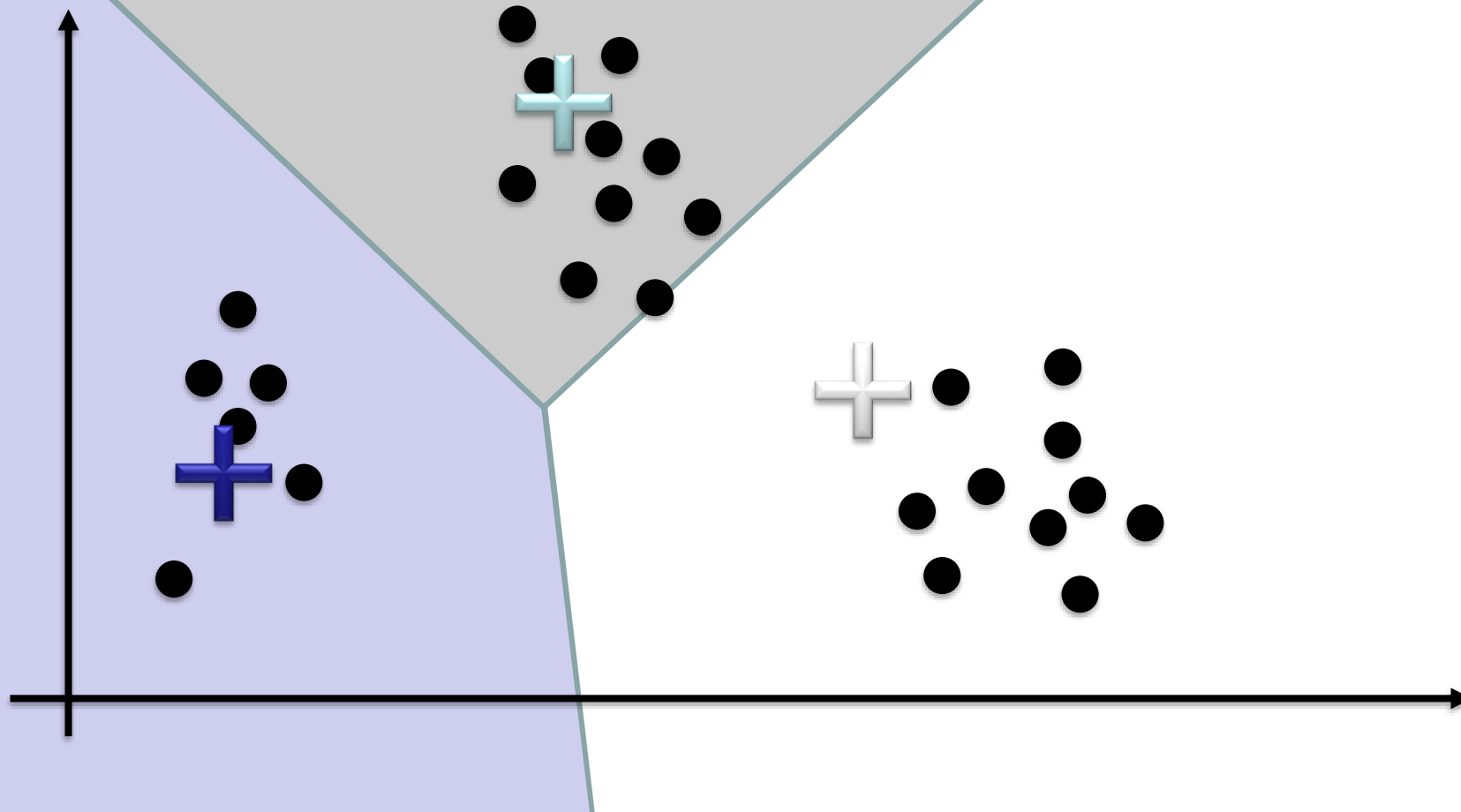
# K-Means Clustering: *Intuition*

- Improved?
- Repeat



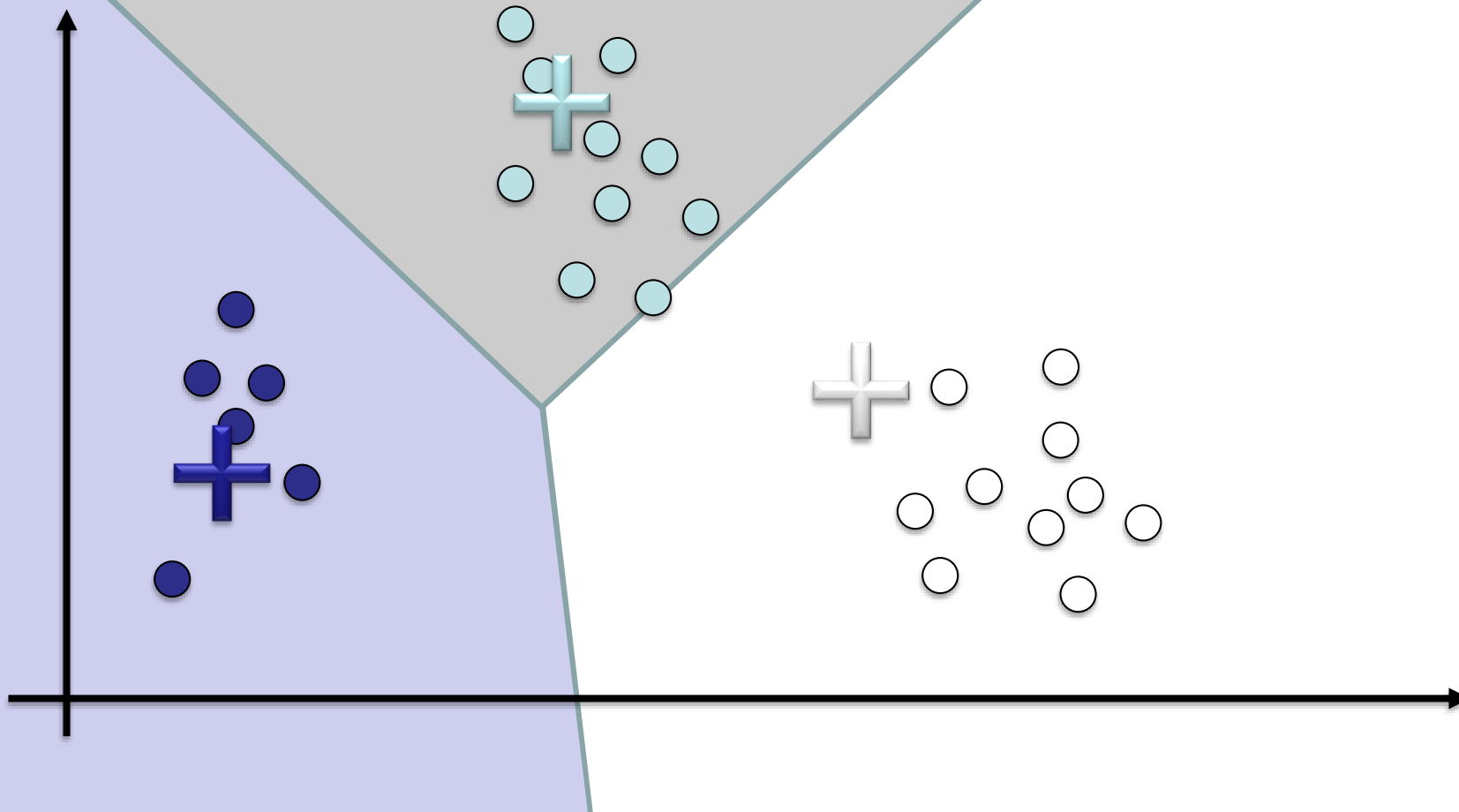
# K-Means Clustering: *Intuition*

- Assign Points



# K-Means Clustering: *Intuition*

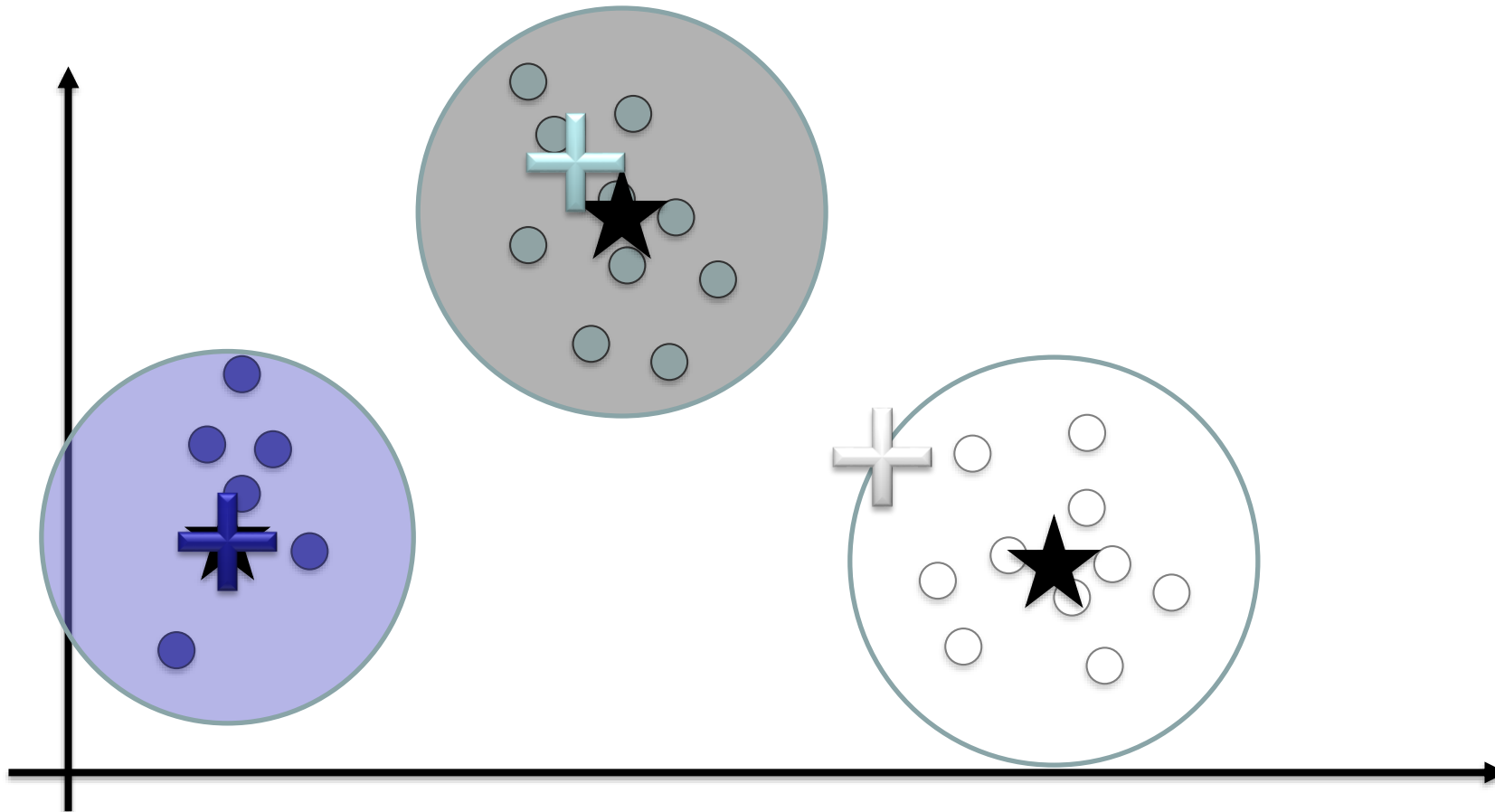
- Assign Points





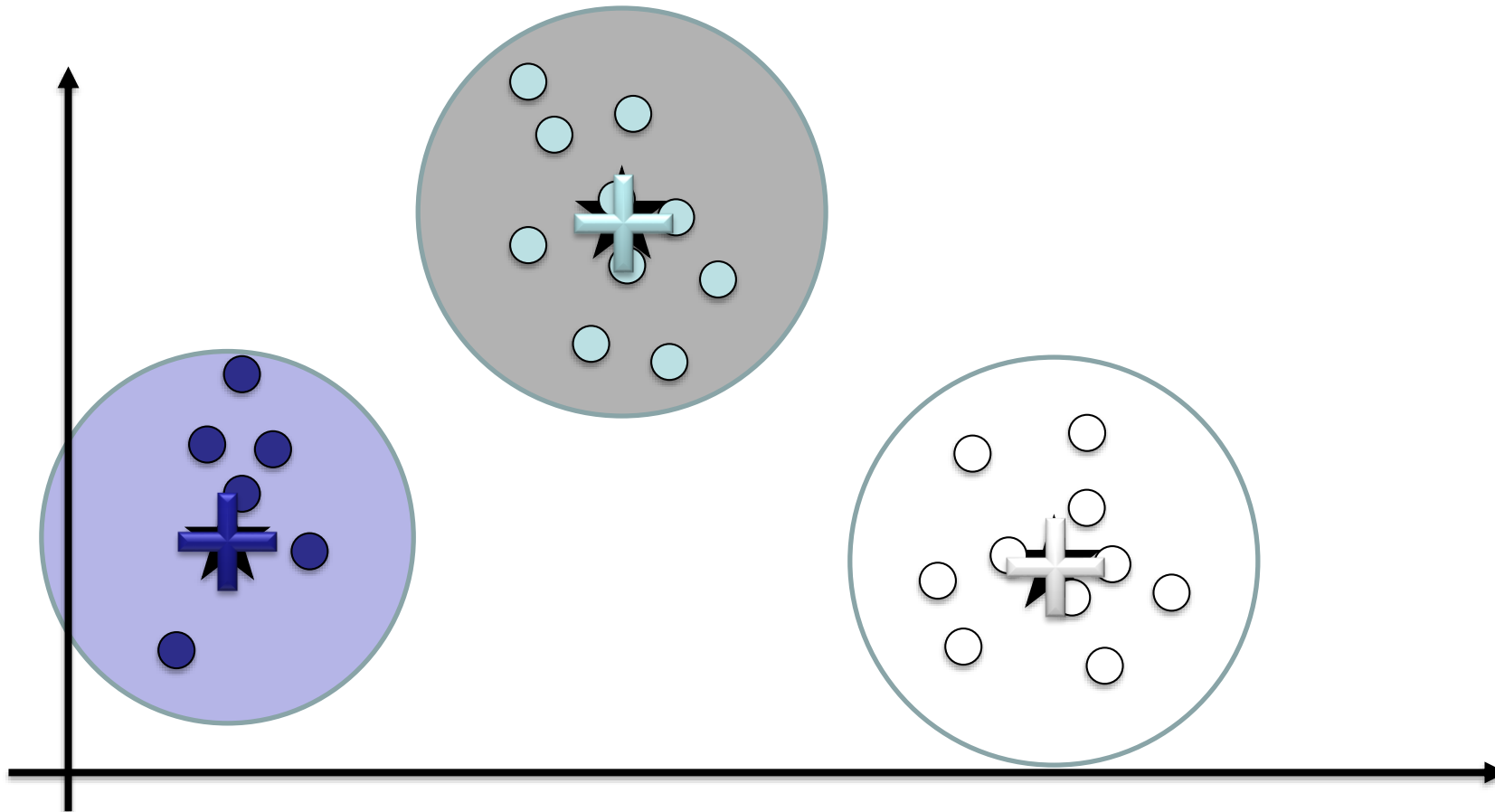
# K-Means Clustering: *Intuition*

- Compute cluster means



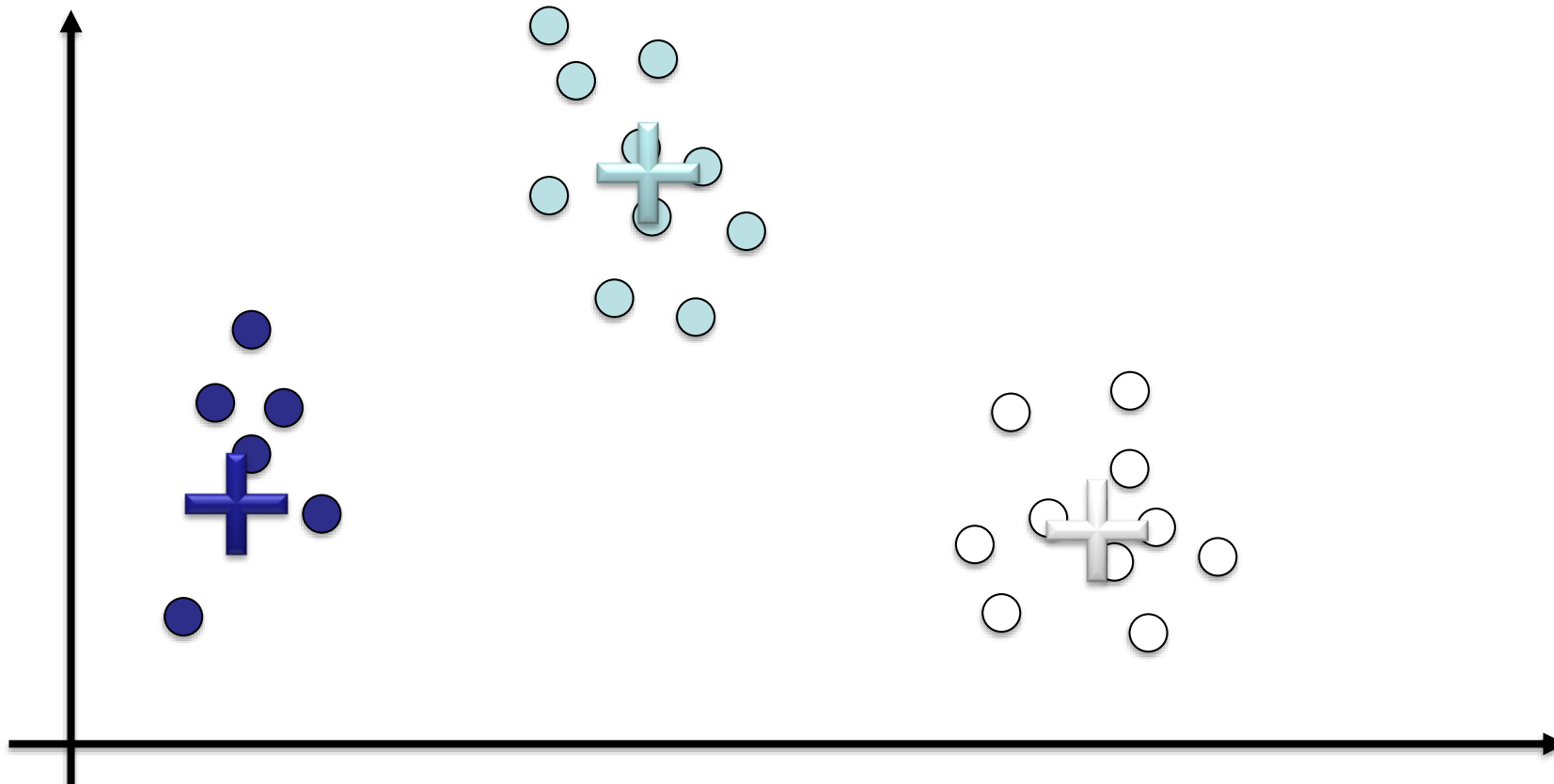
# K-Means Clustering: *Intuition*

- Update cluster centers



# K-Means Clustering: *Intuition*

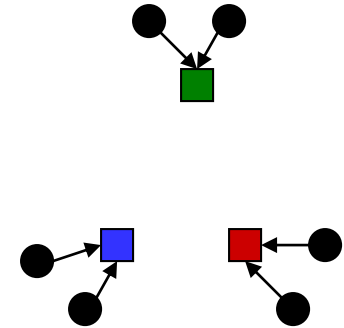
- Repeat?
  - Yes to check that nothing changes → Converged!



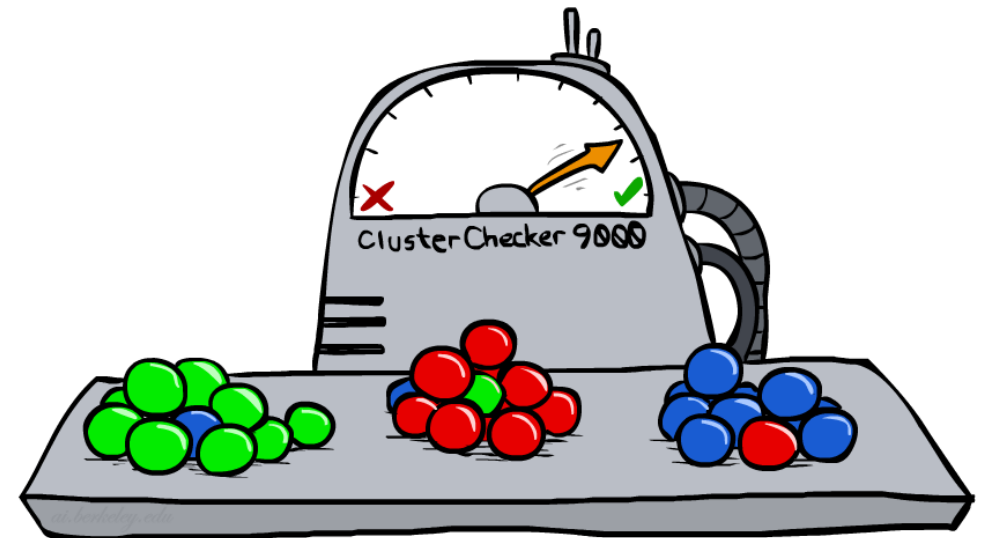
# K-Means as Optimization

- Consider the total distance to the means:

$$\phi(\underbrace{\{x_i\}}_{\text{points}}, \underbrace{\{a_i\}}_{\text{assignments}}, \underbrace{\{c_k\}}_{\text{means}}) = \sum_i \underbrace{\text{dist}(x_i, c_{a_i})}_{\text{squared Euclidean distance}}$$



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



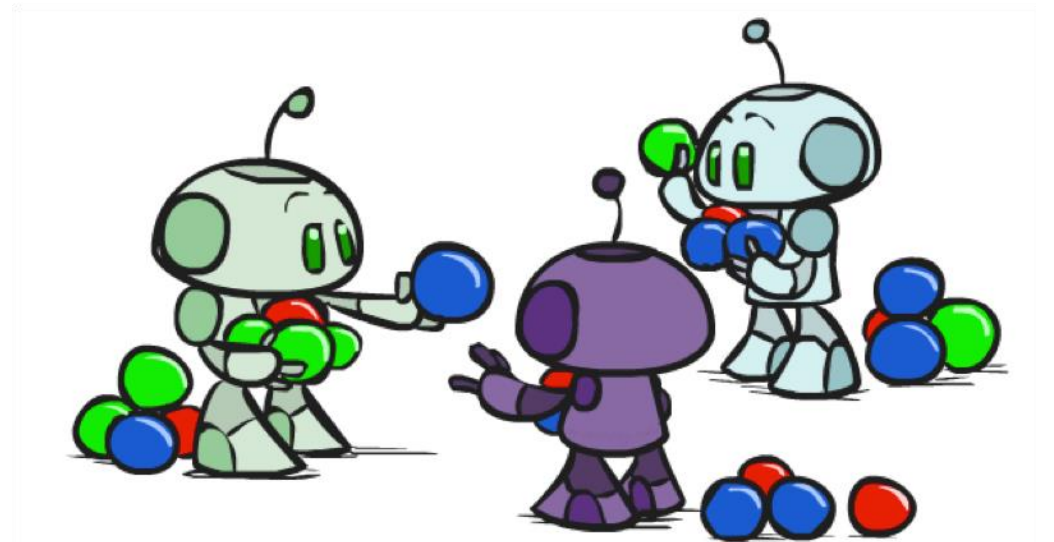
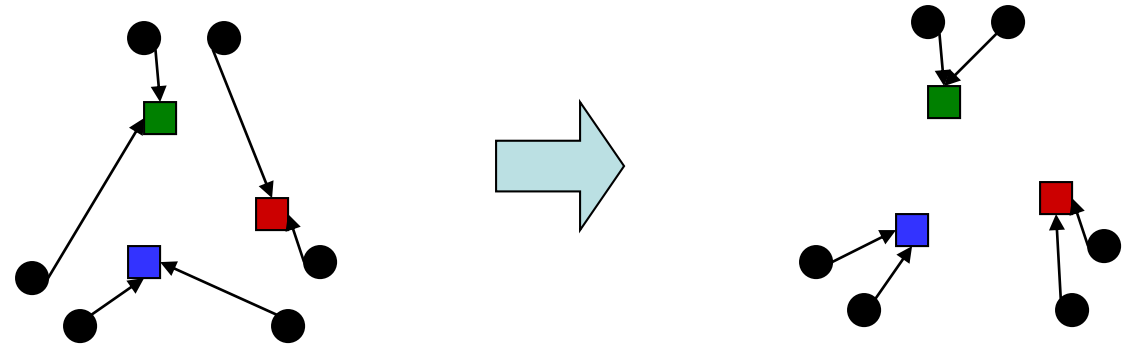
# Phase I: Update Assignments

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

$$a_i = \operatorname{argmin}_k \text{dist}(x_i, c_k)$$

- Cannot increase total distance phi!

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

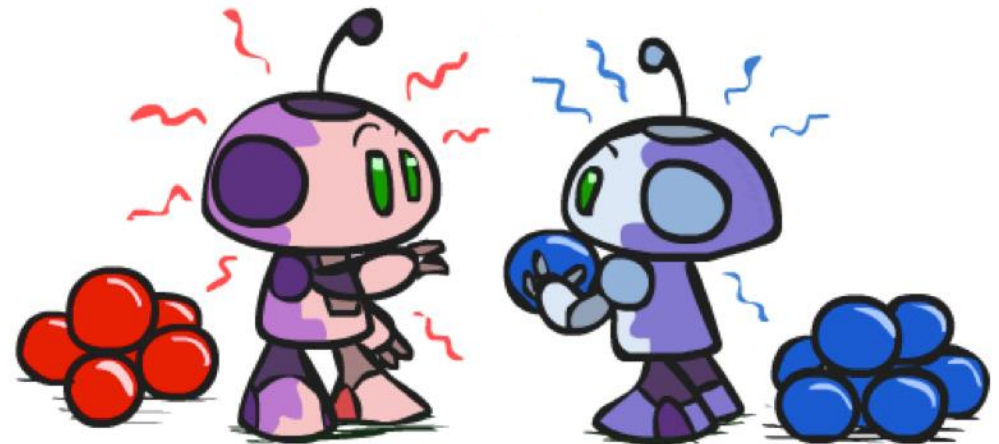
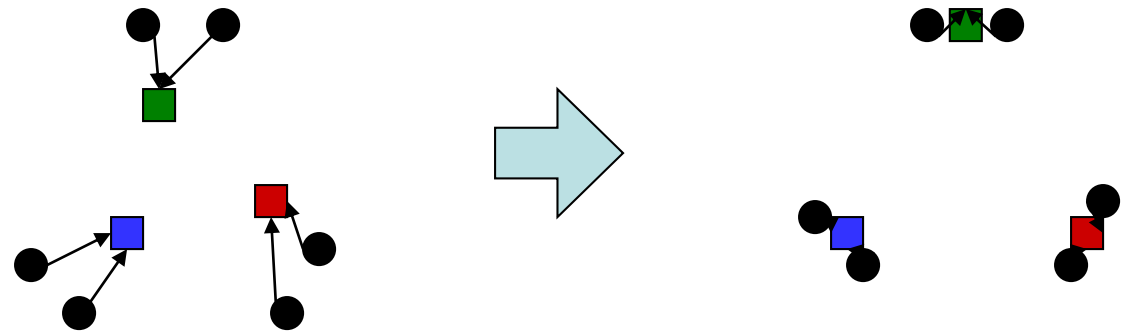


# Phase II: Update Means

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

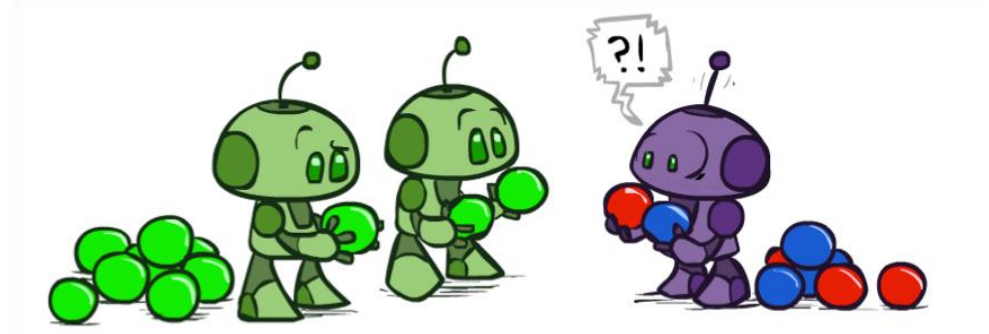
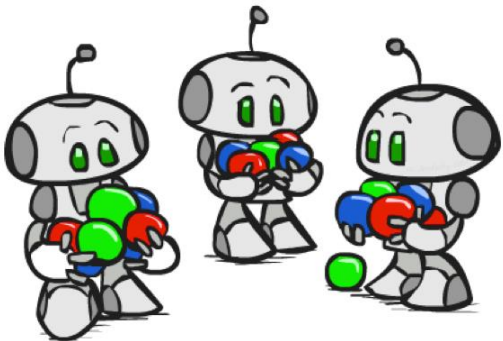
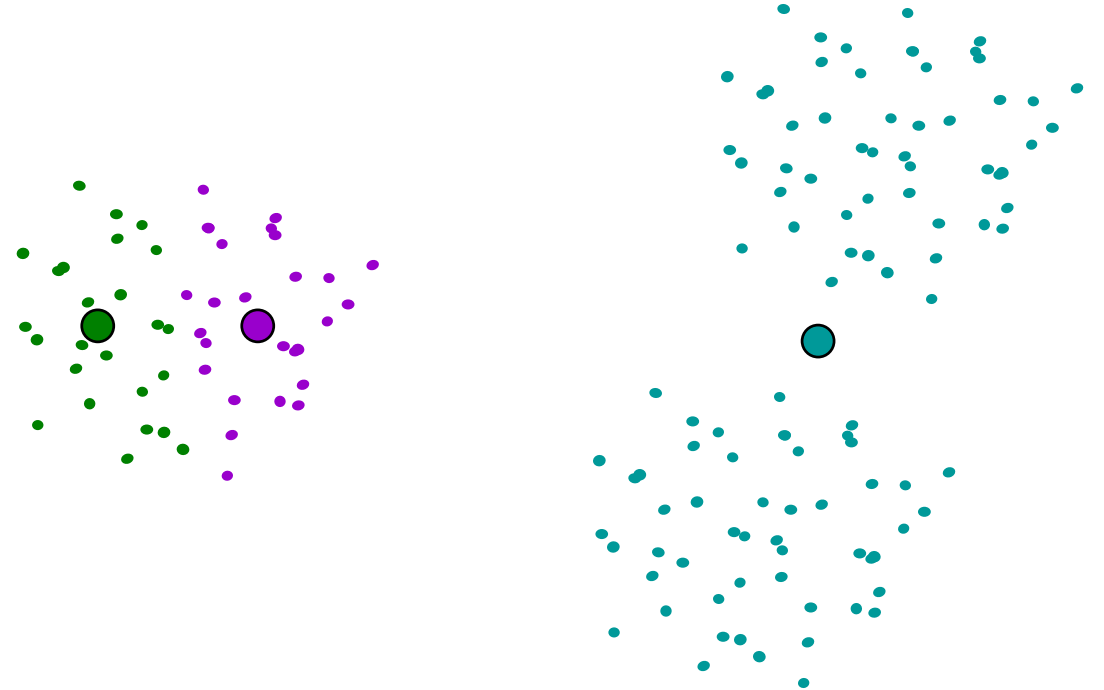
$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

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

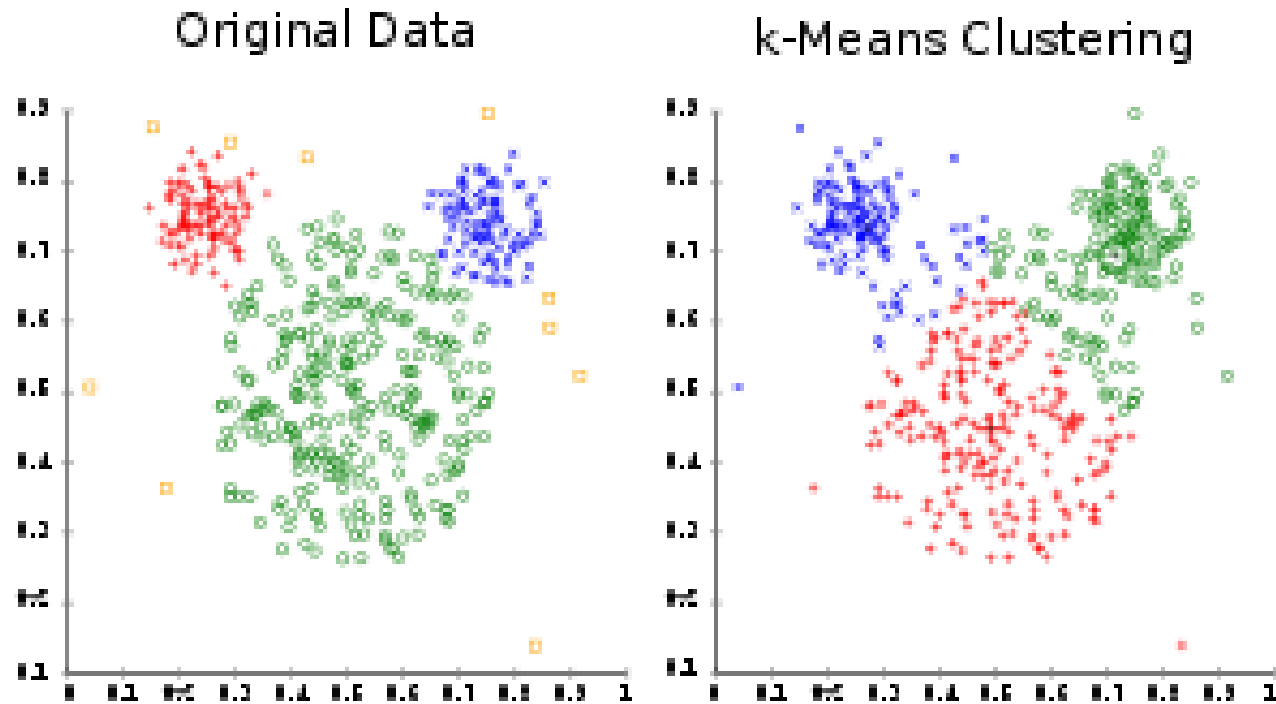


# Initialization

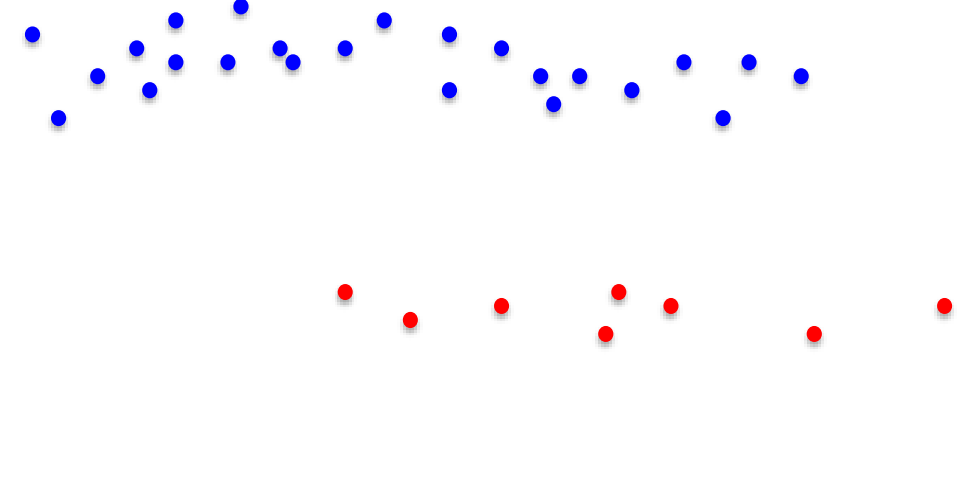
- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
    - Local optima



# Inductive Bias



Equally Sized Clusters



Circular Clusters



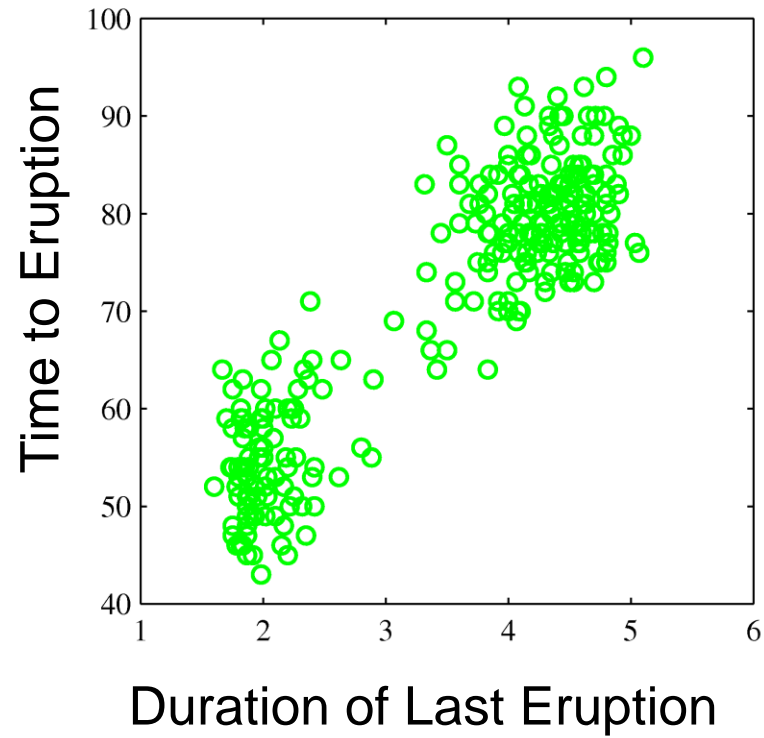
# Probabilistic Clustering

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- Try a probabilistic model!
  - allows overlaps, clusters of different sizes/shapes, etc.
- Gaussian mixture model (GMM)
  - also called Mixture of Gaussians

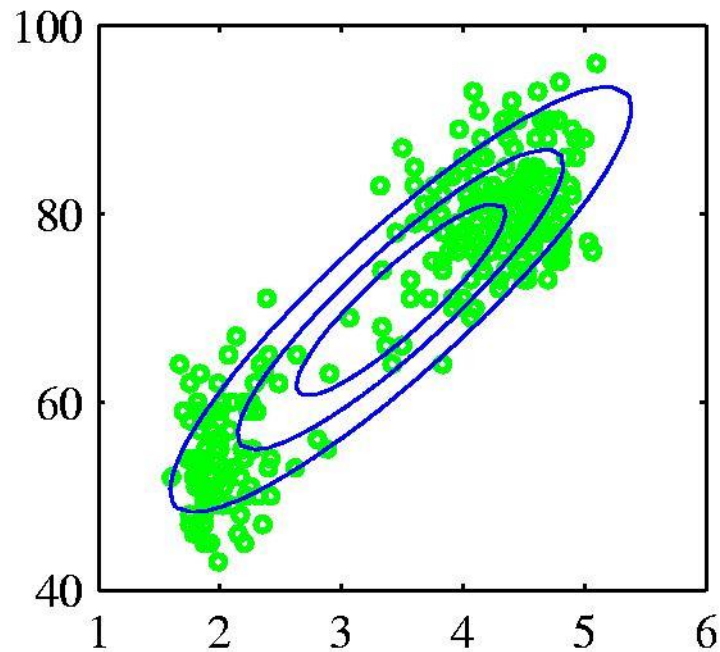
# Mixtures of Gaussians

- Old Faithful Data Set

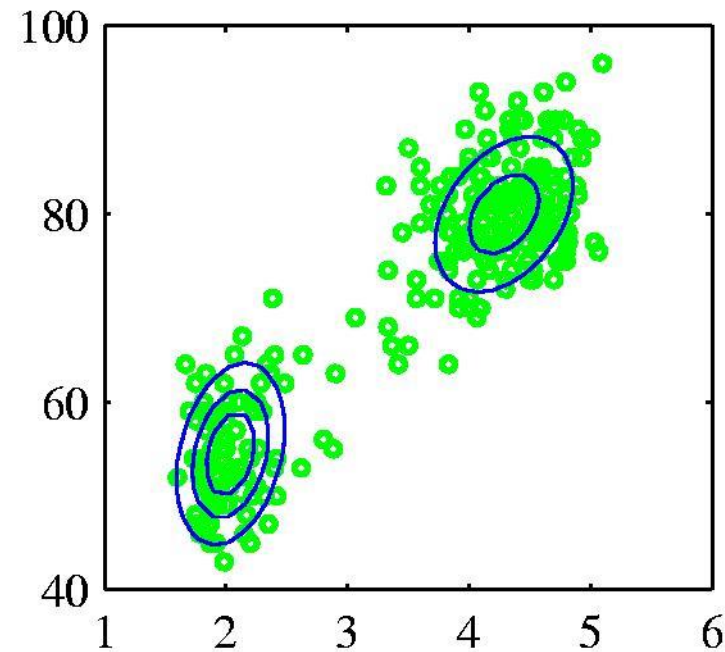


# Mixtures of Gaussians

- Old Faithful Data Set



Single Gaussian



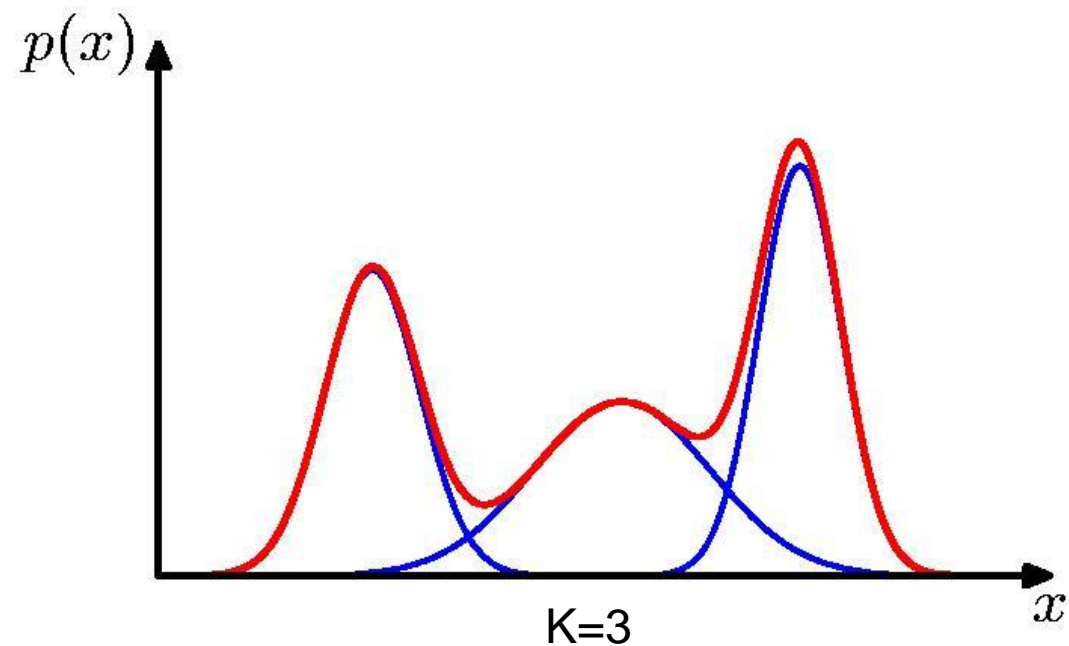
Mixture of two  
Gaussians

# Mixtures of Gaussians

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \underbrace{\mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

Mixing coefficient

$$\forall k : \pi_k \geq 0 \quad \sum_{k=1}^K \pi_k = 1$$

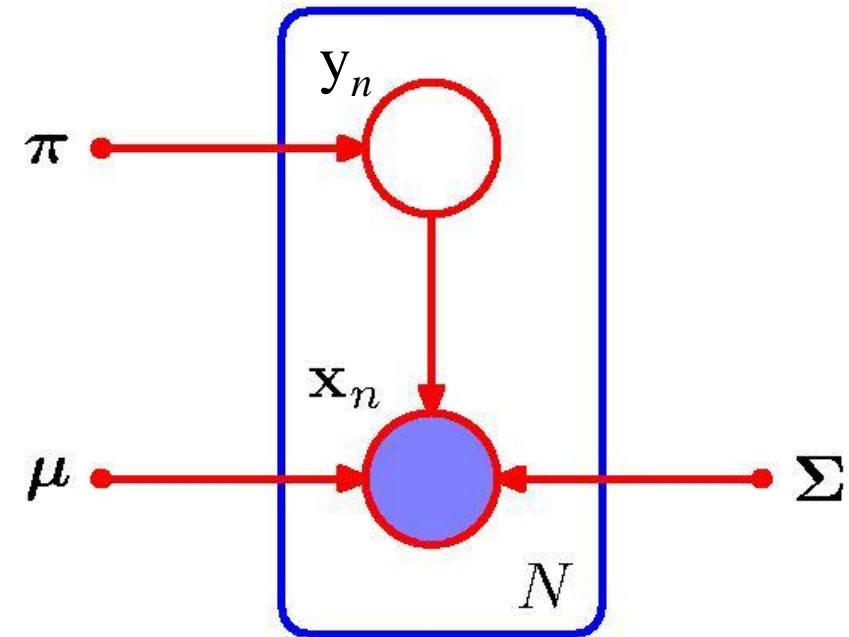


# Gaussian mixture model

- $P(Y)$ : Distribution over  $k$  components (clusters)
- $P(X|Y)$ : Each component generates data from a **multivariate Gaussian** with mean  $\mu_i$  and covariance matrix  $\Sigma_i$

Each data point is sampled from a  
***generative process***:

1. Choose component  $i$  with probability  $\pi_i$
2. Generate data point from  $N(\mathbf{x} | \mu_i, \Sigma_i)$

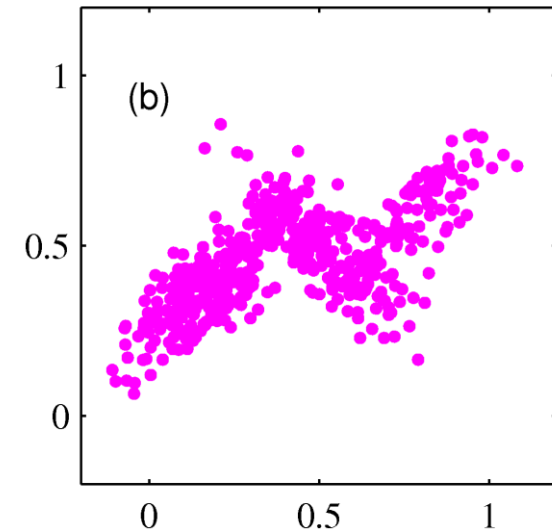


# Unsupervised learning for GMM

- In clustering, we don't know the labels  $Y$ !
- Maximize marginal likelihood:

$$\prod_j P(\mathbf{x}_j) = \prod_j \sum_i P(y_j = i, \mathbf{x}_j) = \prod_j \sum_i \pi_i N(\mathbf{x}_j | \mu_i, \Sigma_i)$$

- How do we optimize it?
  - No closed form solution



# Expectation Maximization (EM)

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- Pick K random cluster models (Gaussians)
- Alternate:
  - Assign data instances **proportionately** to different models
  - Revise each cluster model based on its (**proportionately**) assigned points
- Stop when no changes

# EM: Two Easy Steps

**Objective:**  $\operatorname{argmax}_{\theta} \prod_j \sum_{i=1}^k P(y_j=i, x_j | \theta) = \sum_j \log \sum_{i=1}^k P(y_j=i, x_j | \theta)$

**Data:**  $\{x_j \mid j=1 \dots n\}$

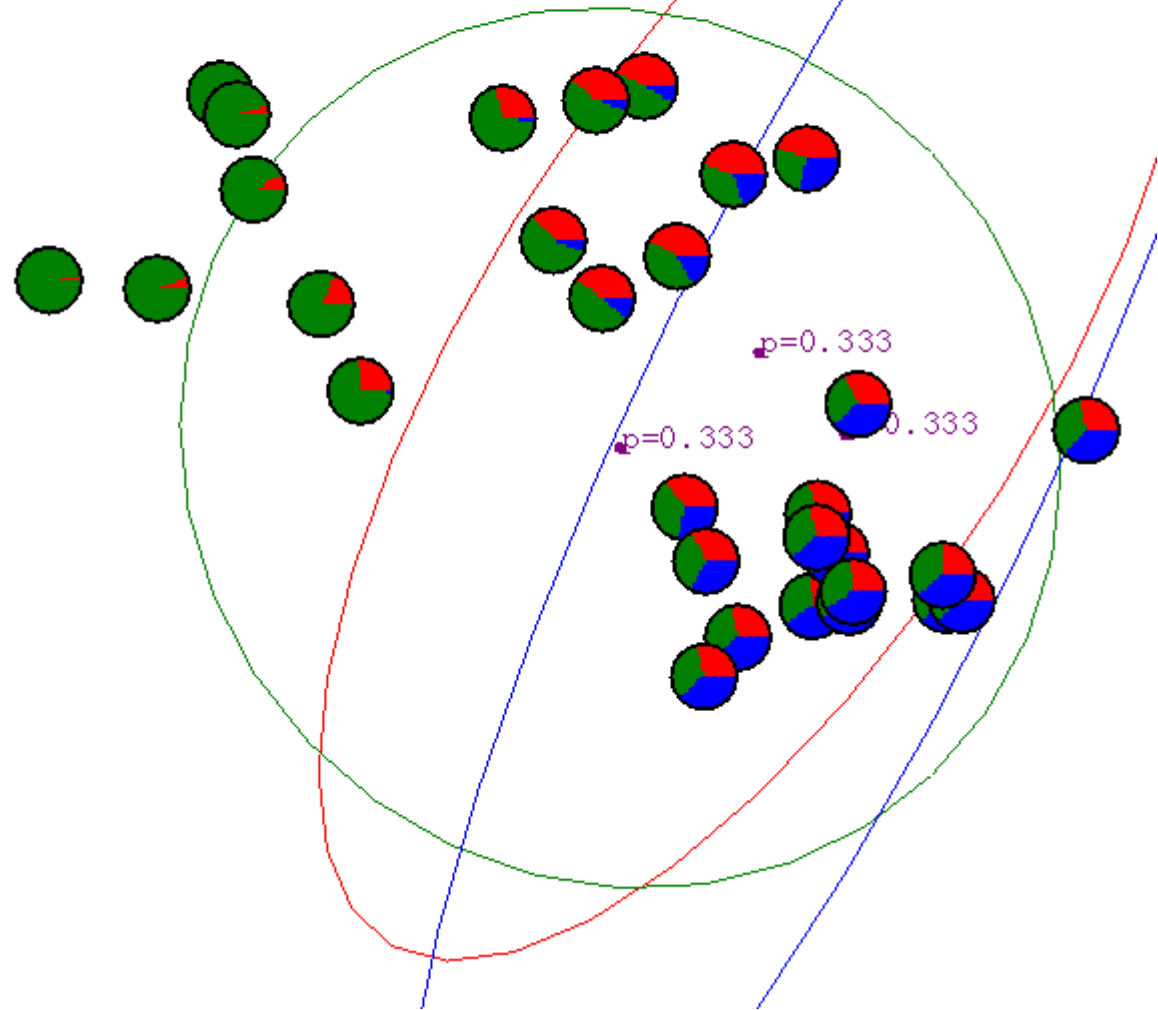
Notation a bit  
inconsistent  
Parameters =  $\theta = \lambda$

- **E-step:** Compute expectations to “fill in” missing  $y$  values according to current parameters,  $\theta$ 
  - For all examples  $j$  and values  $i$  for  $y$ , compute:  $P(y_j=i \mid x_j, \theta)$
- **M-step:** Re-estimate the parameters with “weighted” MLE estimates
  - Set  $\theta = \operatorname{argmax}_{\theta} \sum_j \sum_{i=1}^k P(y_j=i \mid x_j, \theta) \log P(y_j=i, x_j | \theta)$

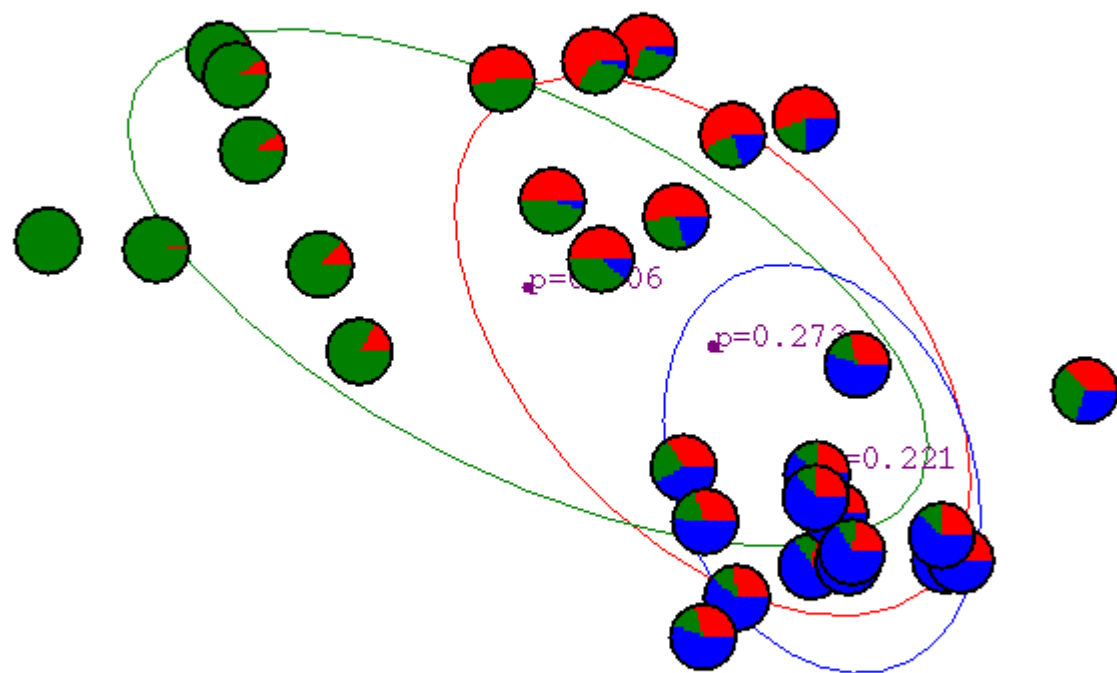
Especially useful when the E and M steps have closed form solutions!!!



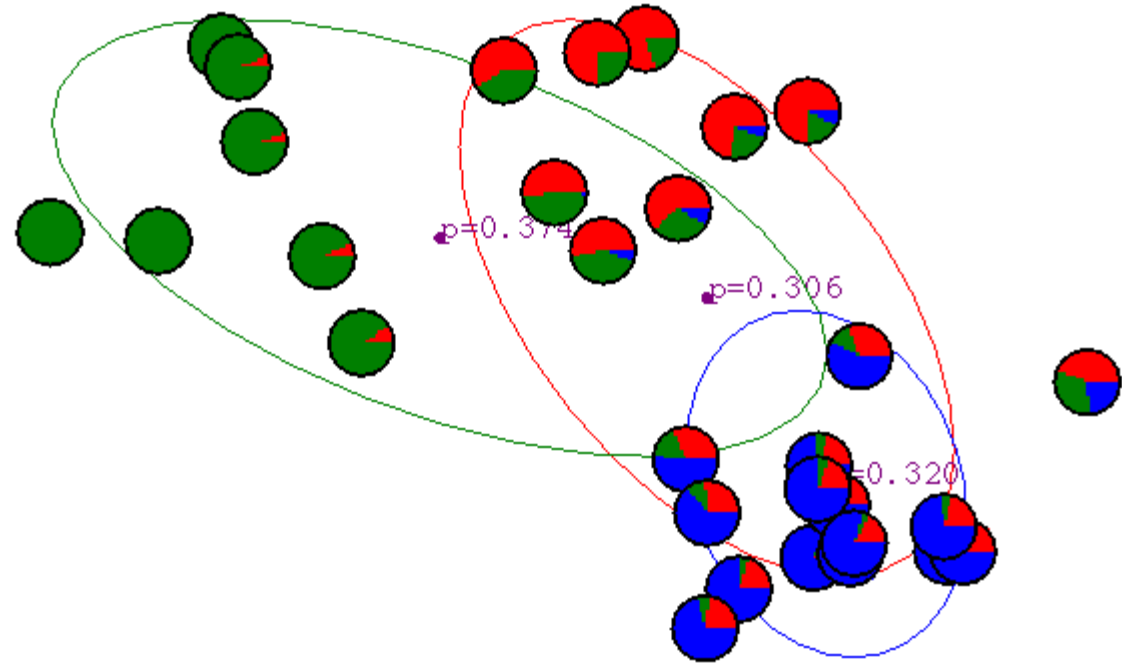
# Gaussian Mixture Example: Start



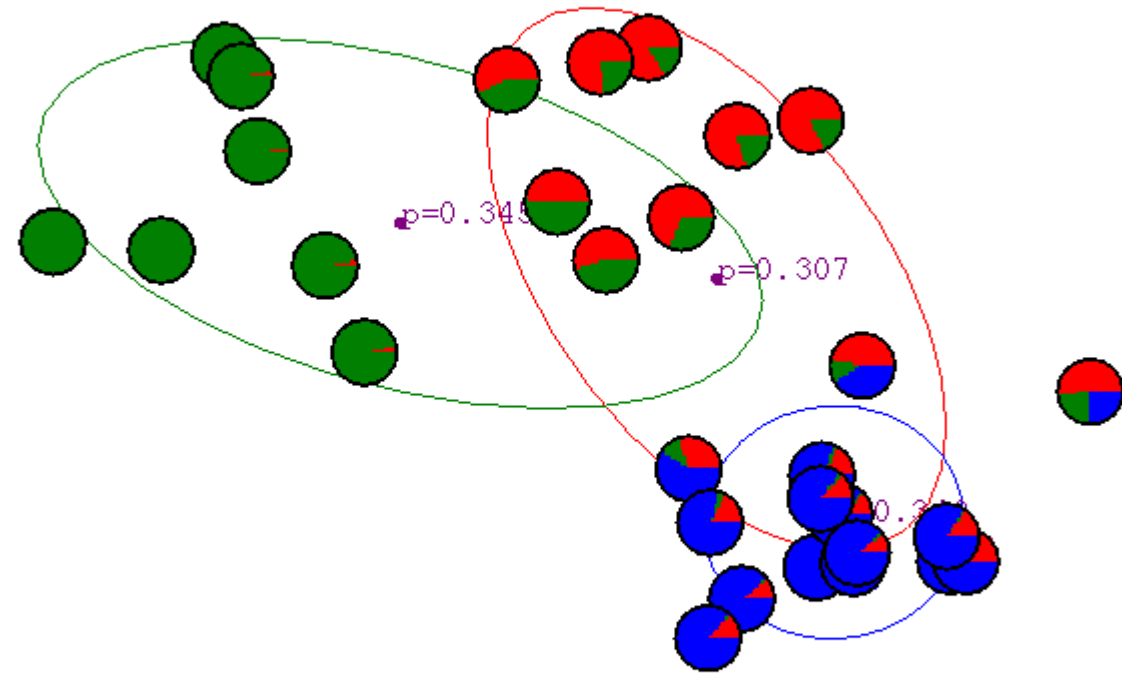
# After first iteration



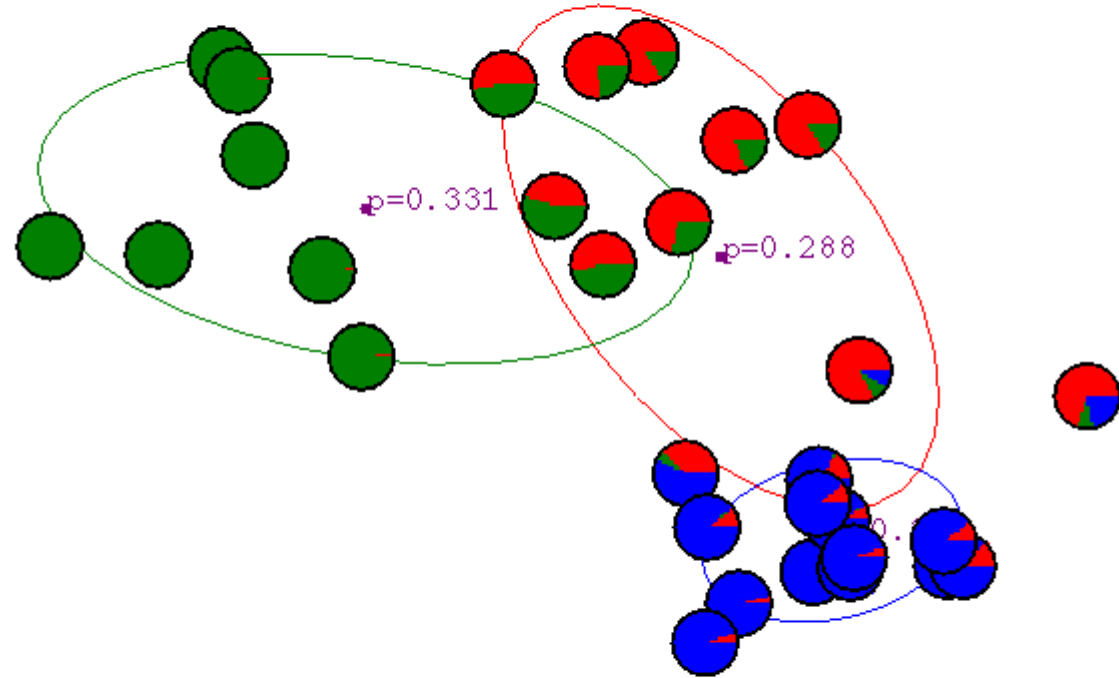
# After 2nd iteration



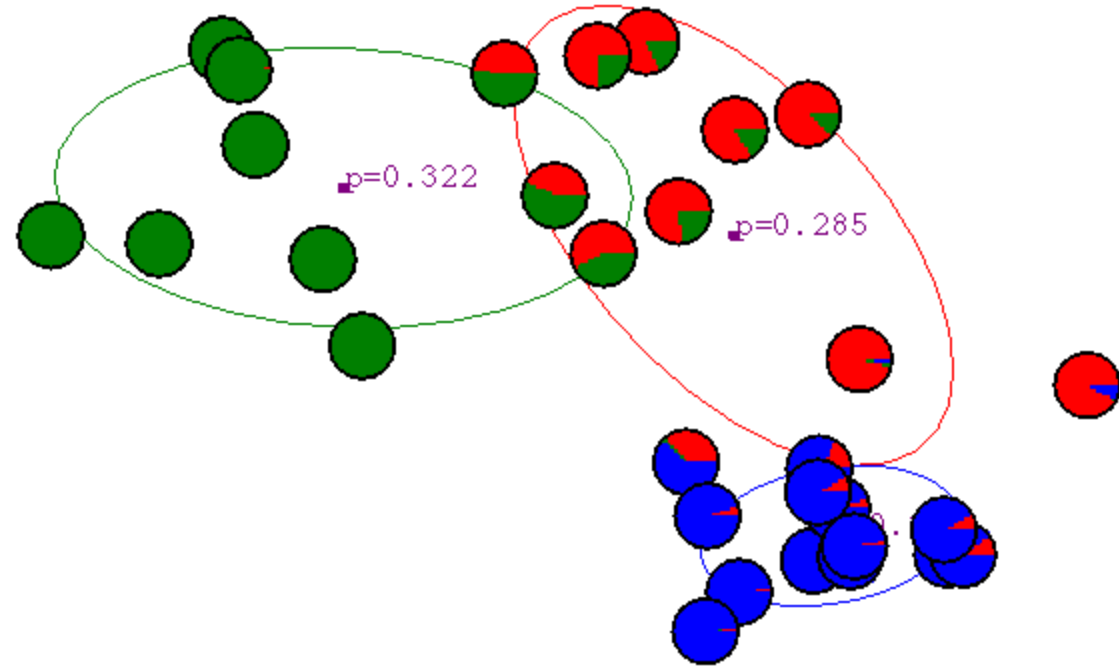
# After 3rd iteration



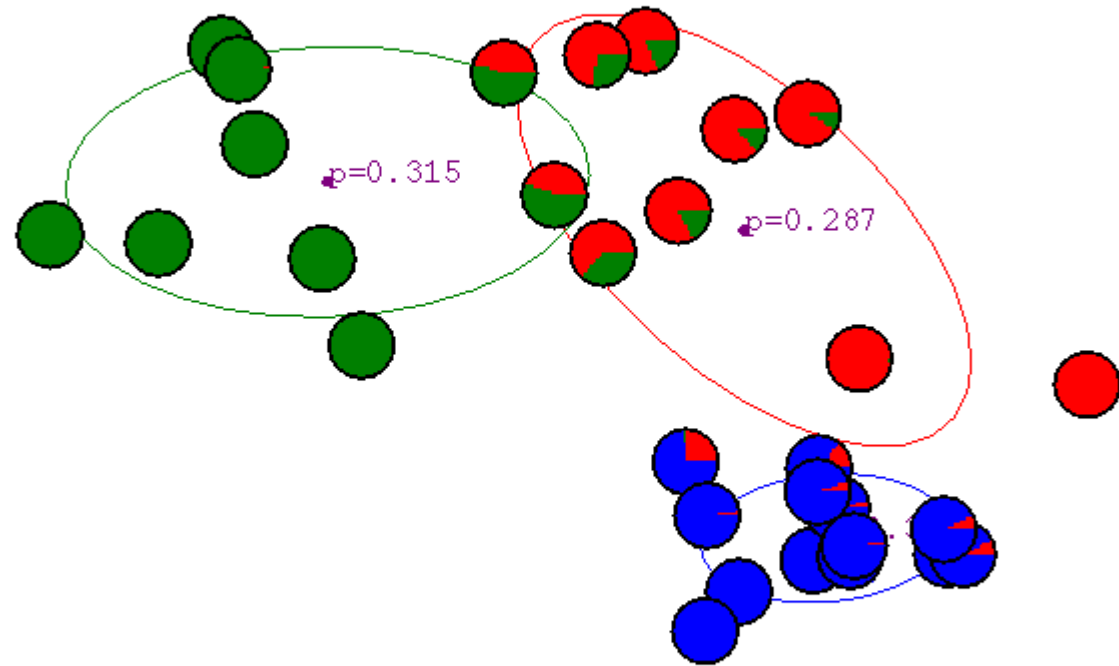
# After 4th iteration



# After 5th iteration

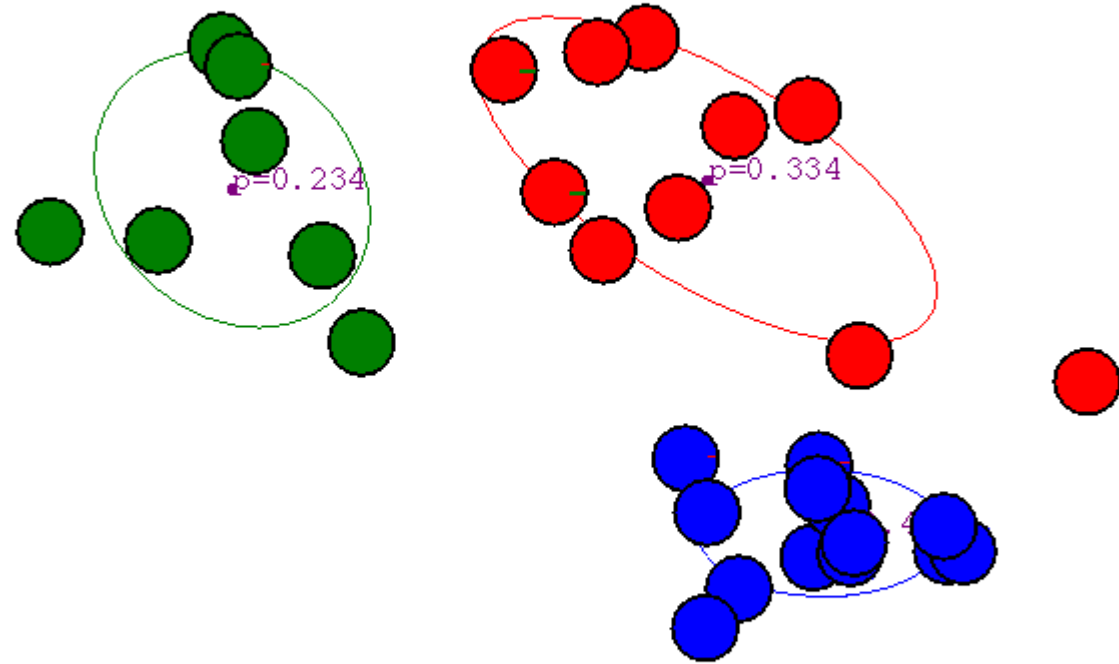


# After 6th iteration



# After 20th iteration

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# EM and K-means

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- EM degrades to k-means if we assume
  - All the Gaussians are spherical and have identical weights and covariances
    - i.e., the only parameters are the means
  - The label distributions computed at E-step are point-estimations
    - i.e., hard-assignments of data points to Gaussians
    - Alternatively, assume the variances are close to zero

# EM in General

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- Can be used to learn any model with hidden variables (missing data)
- Alternate:
  - Compute distributions over hidden variables based on current parameter values
  - Compute new parameter values to maximize expected log likelihood based on distributions over hidden variables
- Stop when no changes

# Summary

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- Clustering

- Group together similar instances

- K-means

- Assign data instances to closest mean
  - Assign each mean to the average of its assigned points

- EM

- Assign data instances proportionately to different Gaussian models
  - Revise each model based on its (proportionately) assigned points