A2 Overview

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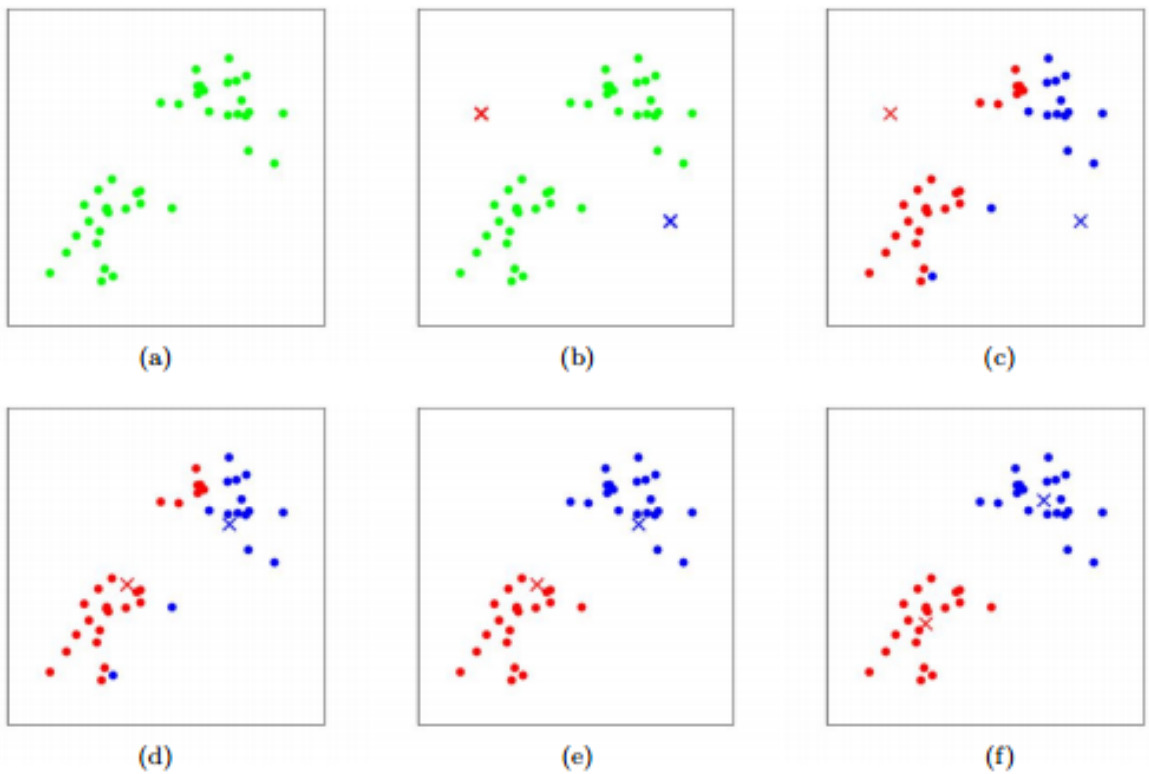
Two MPI Problems

1. Heat Simulation
2. K-means clustering

Previously discussed strategies to parallelize heat problem for distributed memory machine in lecture, will discuss K-Means now

K-Means Clustering

- A standard ML / Data Mining / Stats problem
- Input: data + #of clusters desired
- Output: assignment of each data to a cluster + cluster centers
- Algorithm: Iterates between
  1. Calculate cluster centers
  2. Calculate cluster assignments



Source: K-Means by Chris Piech. Based on a handout by Andrew Ng.

Overall

```
# ASSIGN RANDOM CLUSTER TO EACH DATA
...

maxiter = 100        # bounds the iterations
curiter = 1          # current iteration
nchanges = ndata     # count changes in assignment each iter

while nchanges > 0 and curiter <= maxiter: # loop until convergence
  # DETERMINE NEW CLUSTER CENTERS
  ...

  # DETERMINE NEW CLUSTER ASSIGNMENTS FOR EACH DATA
  ...
```

Initial Assignment to Random Clusters

```
1   for i in range(data.ndata):          # random, regular initial cluster assign
2     c = i % clust.nclust
3     data.assigns.append(c)
4
5   for c in range(clust.nclust):
6     icount = data.ndata / clust.nclust;
7     extra = 0
8     if c < (data.ndata % clust.nclust):
9       extra = 1                        # extras in earlier clusters
10    clust.counts[c] = icount + extra;
```

Determine Cluster Centers

```
1  # DETERMINE NEW CLUSTER CENTERS
2  for c in range(clust.nclust):       # reset cluster centers to 0.0
3    for d in range(clust.dim):
4      clust.features[c][d] = 0.0
5
6  for i in range(data.ndata):         # sum up data in each cluster
7    c = data.assigns[i]
8    for d in range(clust.dim):
9      clust.features[c][d] += data.features[i][d]
10
11 for c in range(clust.nclust):       # divide by ndatas of data to
12   if clust.counts[c] > 0:           # get mean of cluster center
13     for d in range(clust.dim):
14       clust.features[c][d] = clust.features[c][d] / clust.counts[c]
```

Determine Cluster Assignments

```
# DETERMINE NEW CLUSTER ASSIGNMENTS FOR EACH DATA
for c in range(clust.nclust):       # reset cluster counts to 0
  clust.counts[c] = 0

nchanges = 0
for i in range(data.ndata):         # iterate over all data
  best_clust = None
  best_distsq = float("inf")
  for c in range(clust.nclust):     # compare data clusters, assign closest
    distsq = 0.0
    for d in range(clust.dim):      # calculate squared distance to each dim
      diff = data.features[i][d] - clust.features[c][d]
      distsq += diff*diff
    if distsq < best_distsq:        # if closer to this cluster than
      best_clust = c                # current best
      best_distsq = distsq
  clust.counts[best_clust] += 1
  if best_clust != data.assigns[i]:  # assigning data to a different cluster?
    nchanges += 1                    # indicate cluster assignment has changed
    data.assigns[i] = best_clust     # assign to new cluster
```

Distributed Memory Parallel Versions

- Algorithm deals with Data and Clusters, each a matrixy thing
- How would you divide up this data in a distributed parallel version?
- Would data redistribution be required in your scheme?
- What information needs to be exchanged at each iteration?
- Do processors need to communicate for the initial cluster assignment? Or can data be assigned to initial clusters without communication?

Shared Memory Parallel Versions

- Determine which loops Can and Should be parallelized in a shared memory system
- Is any coordination required for loop iterations? Reductions needed?
- Suggest some places to put OpenMP `#pragma` directives