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Center for High-Performance Computing

AI, Machine Learning, and NLP Services at CHPC

Sean Igo
Center for High Performance Computing
Sean.Igo@utah.edu

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Purpose of Presentation

- Brief overview of CHPC environment / access
- Overview of NLP / ML / AI
- Presentation of available NLP/ML/etc software
  - Concentrating on command line utilities on batch-scheduled systems.
    - Interactive software is available

Overview of CHPC Resources

- *CHPC's mission:* ***Support Research!***
  - Faculty, staff, or thesis/dissertation
  - Can also be class research
- CHPC's main focus is High Performance Computing:
  - Massively parallel-processing
  - Remote access to a single high-powered computer
  - Useful for large amounts of data
  - Or if you need an application you don't have

Overview of CHPC Resources

- *Other services available:*
  - VM Farm: web application hosting, grid, etc.
  - Database consultation and hosting
  - Windows/Macs hosted in datacenter, remote login
  - Limited coding/scripting consultation
- My area of expertise is the HPC (cluster) side
  - Suitable for many researchers' needs
  - Ordinary software as well as supercomputing

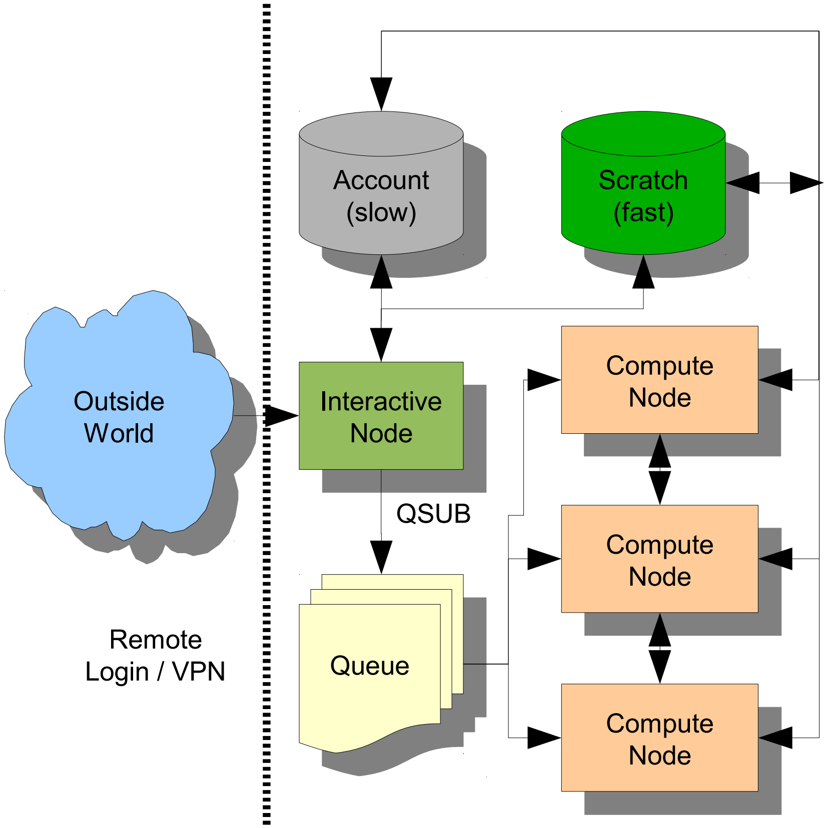
Overview of CHPC Resources

- Protected environment
  - For identifiable, IRB-governed PHI data
  - Like general CHPC environment, but smaller
    - Different home directory
    - Same applications available (linux)
  - Cluster, VM farm, dedicated machines, etc.
  - Higher security: HIPAA compliant, soon other standards
    - Requires VPN connection from off campus
    - Physically secure backups

VMs / Dedicated Machines

- Protected VM farm
  - VMs only for use by PI-approved projects
    - Web-based applications using PHI
    - Remote Desktop access
- Dedicated machines
  - Usually purchased by PI from grant funds
    - Can run any OS
    - Maintained and backed up by CHPC staff

Cluster Environment



Recommended approach:

- Edit/compile on interactive
- Create script for batch
- Submit script to scheduler
- Script does this:
  - Copy data to scratch
  - Process data
  - Write output to scratch
  - Copy output to account
  - Clean up scratch

Getting Started at CHPC

- NOTE: CHPC website is currently under construction
- Links in this presentation may change

Getting Started at CHPC

- Account application
  - online: https://www.chpc.utah.edu/apps/profile/account_request.php
  - You need to be doing research for a PI with a CHPC account
    - If your PI isn't signed up, let me know
  - If the online application is unsuitable, paper one is available
    - www.chpc.utah.edu/docs/forms/application.html
- Protected environment access
  - Application not yet automated
  - Mention in application notes that you need HIPAA/Protected
  - Access based on IRB number

Getting Started at CHPC

- Getting started guide
  - www.chpc.utah.edu/docs/manuals/getting_started
- Problem reporting system
  - Easiest: email to issues@chpc.utah.edu
  - OR go to website http://jira.chpc.utah.edu
  - OR find me

Security Policies (1)

- No clear text passwords - use ssh and scp
- Do not share your account under any circumstances
- Don’t leave your terminal unattended while logged into your account
- Do not introduce classified or sensitive work onto CHPC systems
  - Except in the protected environment
- Use a good password and protect it – see gate.acs.utah.edu for tips on good passwords

Security Policies (2)

- Do not try to break passwords, tamper with files, look into anyone else's directory, etc. – your privileges do not extend beyond your own directory
- Do not distribute or copy privileged data or software
- Report suspicions to CHPC (security@chpc.utah.edu)
- Protected environment data subject to additional policies

General Information

- Available on CHPC web pages
  - https://www.chpc.utah.edu/
- Can get to software info from https://wiki.chpc.utah.edu
  - Again, new site phasing in at the moment
- Available for most packages
  - Can get dated; refer to software homepages
- Has information on licensing restrictions, example batch scripts, where to get more information on a specific package
- Also has useful information on running of jobs

Artificial Intelligence

- The attempt to make computers behave "intelligently"
  - Whatever that means
- A very broad field; practitioners have different aims
  - "problems for which there is no algorithm"
  - modeling of human intelligence (CogSci)
- CHPC use to date has been application-oriented
- **What would you like to hear about?**
  - **these slides are mostly general overview**

Artificial Intelligence

- I will concentrate on simple theory
- Many different subtypes
  - State-space
  - Rule based
  - Logic
  - Classification
  - Clustering
  - Sequencing
  - ...
- Currently mostly means machine learning

Artificial Intelligence

- GENERALLY:
- Many approaches exist to solving problems
- Best way to proceed:
  - Become familiar with different AI techniques
    - (don't need to be expert, just get a feel)
  - Decide which is the best fit for your problem (may be > 1)
  - Develop a representation accordingly
  - Apply the technique
- This is true of both “classical” AI and ML

Artificial Intelligence

- Often, people will choose the algorithm and try to force their application to fit it.
- **Don't do that!**
- AI is faddish:
  - 1980s – neural nets
  - 1990s – Genetic Algorithms
  - 2000s – Support Vector machines
  - 2010s – (not sure yet.)
- All of these have their uses but none is magic

Artificial Intelligence

- The central challenge in AI:

REPRESENTATION!

- How do you describe your problem to be "computable?"
  - able to be operated upon by your chosen algorithm / software?
- I'll demonstrate with Machine Learning (ML)

Quick ML overview

- Common ML task: Supervised Classification
  - Gather a large number of training examples
  - Have human experts classify them
  - Represent as feature vectors
  - ML algorithm trains a model
  - Classify novel instances with the model
- Example: Classifying days wrt whether to play tennis

Machine Learning

- Using data to “train” models by example
- Operates on “instances”: things of interest
  - Patients, customers, sentences, ...
  - You want to know something about the instances, e.g:
  - Patient: likely to be diabetic?
  - Customers: interested in buying Product X?
  - Sentences: relevant to drug interactions?
- Models learned from example instances used to make predictions about new instances

Machine Learning

- Supervised
  - Initial set of example instances given with correct answers
  - Assigned by human experts
  - “gold standard”
- Unsupervised / Semi-supervised
  - No or little human expertise needed
  - Tends to be less reliable and need more data

Feature Engineering

- This is the ML version of representation
- Decide which attributes describe your instances
  - Animals: color, hair length, is_carnivorous,...
  - Patients: age, sex, weight, ...
  - Depends on what you want to find out
- Most of the effort in many ML projects
- A quick example helps to explain...

Quick ML overview

outlook	temperature	humidity	windy	play
sunny	hot	high	FALSE	**no**
sunny	hot	high	TRUE	**no**
overcast	hot	high	FALSE	**yes**
rainy	mild	high	FALSE	**yes**
rainy	cool	normal	FALSE	**yes**
rainy	cool	normal	TRUE	**no**
overcast	cool	normal	TRUE	**yes**
sunny	mild	high	FALSE	**no**
sunny	cool	normal	FALSE	**yes**
rainy	mild	normal	FALSE	**yes**
sunny	mild	normal	TRUE	**yes**
overcast	mild	high	TRUE	**yes**
overcast	hot	normal	FALSE	**yes**
rainy	mild	high	TRUE	**no**

Classic toy ML problem – given the weather, should I play tennis?

(Decision support!)

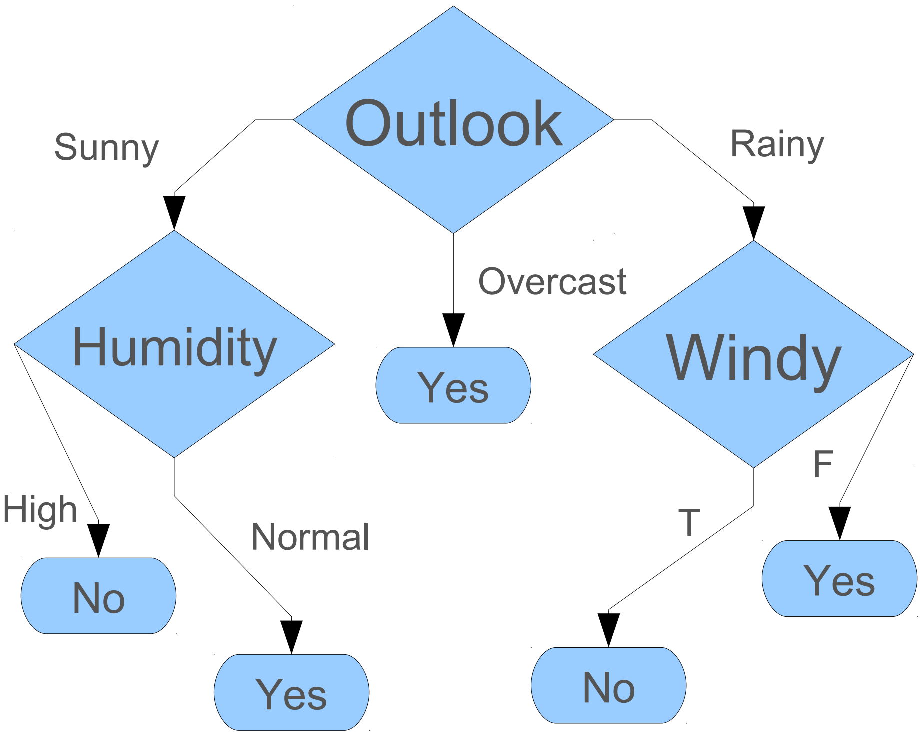
Quick ML overview

```
@relation weather.symbolic

@attribute outlook {sunny, overcast, rainy}
@attribute temperature {hot, mild, cool}
@attribute humidity {high, normal}
@attribute windy {TRUE, FALSE}
@attribute play {yes, no}

@data
sunny,hot,high,FALSE,no
sunny,hot,high,TRUE,no
overcast,hot,high,FALSE,yes
rainy,mild,high,FALSE,yes
rainy,cool,normal,FALSE,yes
rainy,cool,normal,TRUE,no
overcast,cool,normal,TRUE,yes
sunny,mild,high,FALSE,no
sunny,cool,normal,FALSE,yes
rainy,mild,normal,FALSE,yes
sunny,mild,normal,TRUE,yes
overcast,mild,high,TRUE,yes
overcast,hot,normal,FALSE,yes
rainy,mild,high,TRUE,no
```

Convert the examples to file format for the ML software.

Here, Weka ARFF format

Quick ML overview



ML software trains a model

Here, J48 decision tree

```
J48 pruned tree
------------------
outlook = sunny
|   humidity = high: no (3.0)
|   humidity = normal: yes (2.0)
outlook = overcast: yes (4.0)
outlook = rainy
|   windy = TRUE: no (2.0)
|   windy = FALSE: yes (3.0)
```

Decision Tree Classifier

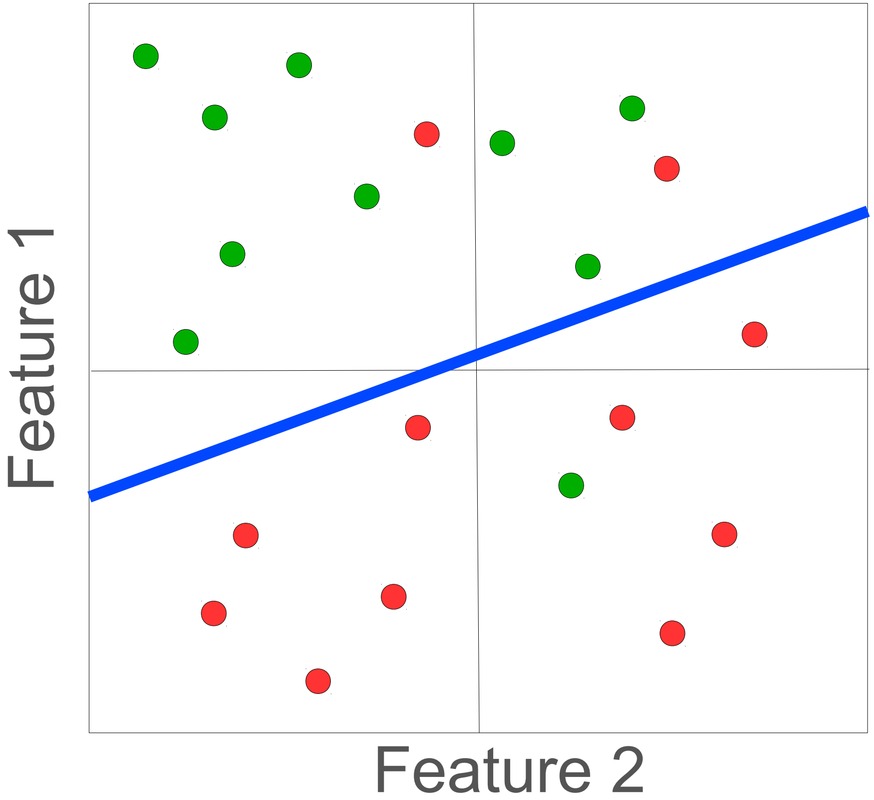
- The type just shown
  - Finds most important feature for discriminating class
  - Creates a branching based on that
  - Does this recursively, creating a "tree"
  - Can also be viewed as a set of rules
- Advantage is that tree / rules human readable
- May not be the best for a given application

Other Classifiers: SVM

- Support Vector Machine
  - treats instances as points on a graph
  - each feature represents a dimension (may be many)
  - finds boundaries separating the classes
    - to the best of its ability
- Default is “linear kernel”
  - Boundary is a line
  - really, multidimensional plane in # features...

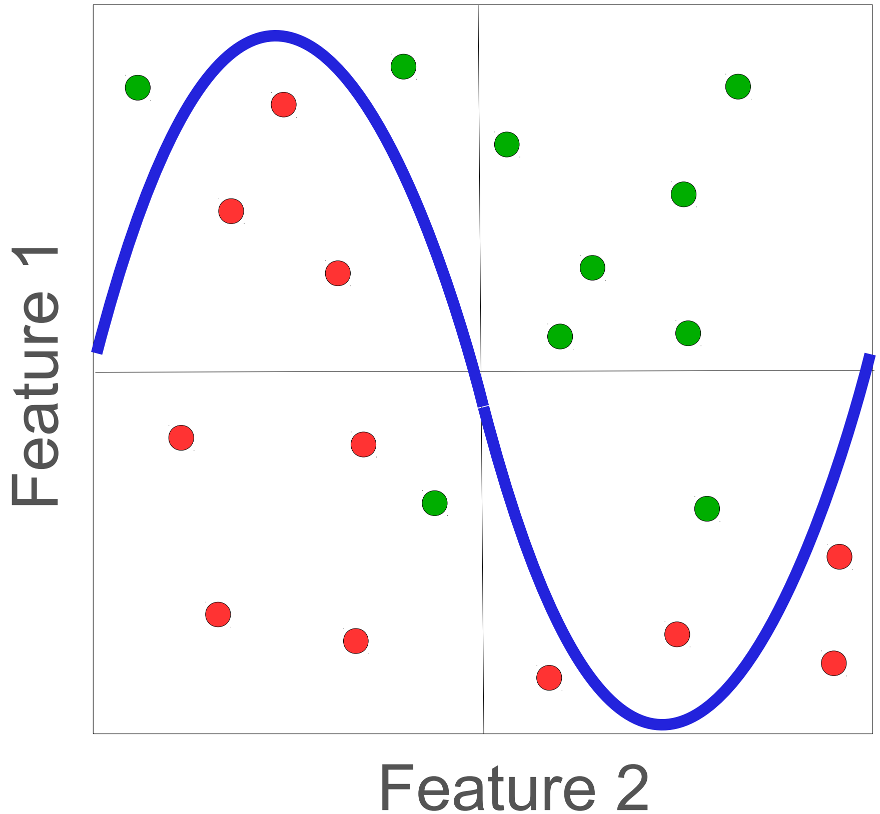
Other Classifiers: SVM

- linear kernel, 2 features, 2 classes (red/grn)



Other Classifiers: SVM

- polynomial kernel order 3, 2 features, 2 classes



Other Classifiers: Naive Bayes

- Uses Bayes' Rule
  - Find probability that an instance belongs to class n
  - Given its combination of features
  - Simplification: Assumes all features are independent
  - Often that's close enough
  - Depends on feature engineering

Classifiers: For best results

- Keep number of classes small
  - Ideally, 2
  - For multi-class can use multiple 2-class classifiers
    - A or not-A, B or not-B, etc.
    - Combine predictions through various means
  - Some algorithms do well with multiclass (e.g. neural nets)
- Best if # of instances of each class ~equal
  - Often not true
  - Depends on feature engineering

Evaluating Classifiers

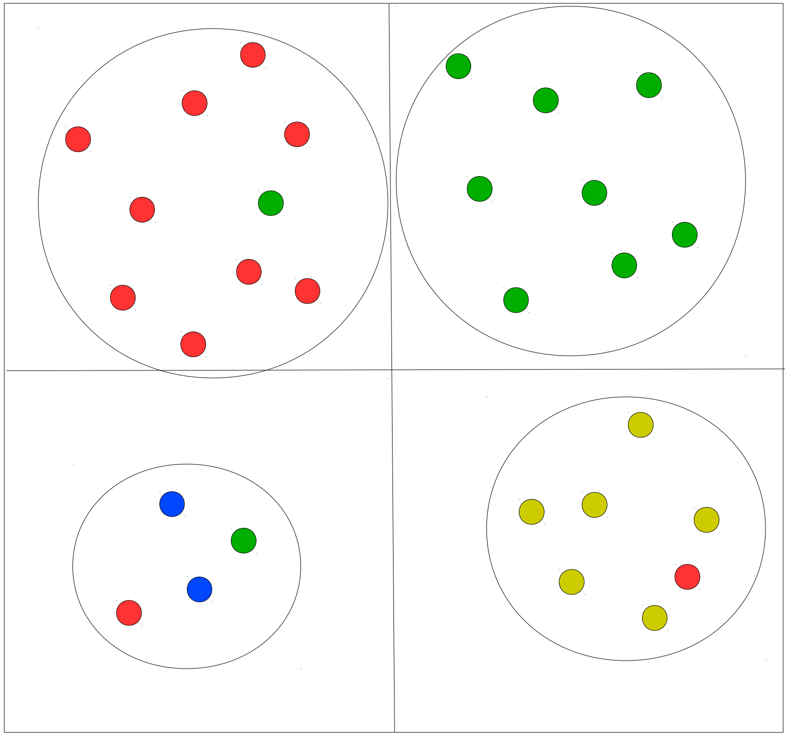
- Supervised
  - With respect to class n
  - Recall: # correct predictions / # of class n in gold standard
  - Precision: # correct predictions / # of total predictions made
  - F-measure: harmonic mean of Recall and Precision
  - Recall aka Sensitivity; Precision = Positive Predictive Value
  - Other metrics exist; R/P/F is common and informative
- Unsupervised
  - Need a different metric... Possibly clustering?

Clustering

- Similar to classification
- Typically unsupervised
  - Can use a gold standard to evaluate cluster purity
- Gather instances into “clusters” by similarity
  - trick is to define similarity
- Different methods:
  - Fixed # clusters
  - Flexible #, e.g. Go until all instances clustered
  - Clusters may overlap or not

Clustering

- Here, fixed 4 clusters (4 classes) – can evaluate w/gold std.



Association Mining

- Looks for patterns of association
- Typically unsupervised
- Find instances that often occur together
  - e.g. in department store data:
  - People who buy baby formula often buy diapers
  - Examples: shopping websites' “you might like”
  - Feedback e.g. customer can click “not interested”

Sequence Finding

- Given n samples in order, predict next
- OR given a sequence, find likelihood it conforms to a model
- Techniques:
  - Conditional Random Fields (CRF)
  - Hidden Markov Models (HMM)
  - ...

So now what?

- There are many more AI techniques
- These have been some of the common ones
  - and the ones I know best
- Moving now to discussing how to use AI / ML

Feature Extraction

- Converting input data to ML software format
- Capturing / synthesizing the features you need
- Input data can be
  - files – text, xml, EHR, ...
  - instrument signals – ECG, Audio...
  - multiple sources
- Output format depends on ML software
  - Common ones: CSV, Weka ARFF

Feature Extraction

- Can be an unexpectedly large software development effort and/or deployment!
  - Be sure to allow time for it in development
- Input data may be difficult to interpret
  - May contain garbage e.g. Email headers
  - A common problem in NLP...
  - May be in undocumented format
- Input and output data may be large
  - Feature extraction takes longer than expected

Typical ML workflow: development

- Decide on representation (feature engineering)
- Gather data / create gold standard
  - Can be time-consuming and expensive!
  - Not as bad for unsupervised methods
- Extract features to make training set / test set
  - Again, different for unsupervised tasks?
- Train model on training set
- Evaluate model against test set
  - Or other metrics e.g. For clustering

Typical ML workflow: deployment

- Export trained model
- Create production software incorporating:
  - Feature extraction methods
  - Prediction method based on model
- For each instance software encounters:
  - Extract features
  - Get prediction from model
  - Continue processing

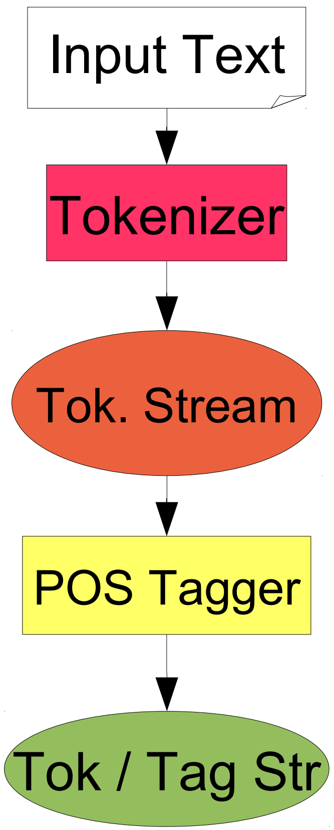
ML Software at CHPC

- Weka
  - Multi-algorithm ML package; java
- SVMLight, SVMLin, SVMLib
- Orange
  - Python extension for ML
- Others: MegaM, VW

NLP Overview

- Application of many AI techniques
- Get computers to understand human language
  - current CHPC software limited to text, not speech
  - also limited to understanding, not generation
- Started in the 1950s
- Turned out to be much harder than it seemed
- Now NLP consists mainly of distinct tasks
  - Some of the most common supported at CHPC

Typical Initial NLP Pipeline




```
The man's dog was brown.
```

```
The, man, 's, dog, was, brown, .
```

```
The_DT, man_NN, 's_POS, dog_NN,
was_VBD, brown_JJ, ._.
```

NLP Software at CHPC

- Stanford Tools:
  - Core, Tagger, NER, Parser
- Berkeley Parser
- Pipeline development: GATE, UIMA
- Sundance (U of U Information extraction)
- Metamap (Biomedical NLP)
- NLTK (Python)

MetaMap – Biomedical NLP

- **`/uufs/chpc.utah.edu/sys/pkg/metamap/std`**
  - Current version metamap10
  - Installed and has java api
- I have done parallelized runs with this
- Same as the online MetaMap utility
- To use, you must sign UMLS agreement

MetaMap – Biomedical NLP

```
Processing 00000000.tx.1: common cold

Phrase: "common cold"
Meta Candidates (6):
  1000 C0009443:Common Cold [Disease or Syndrome]
          Cold
   861 C0009264:Cold (Cold Temperature) [Natural Phenomenon or Process]
   861 C0205214:Common [Functional Concept,Quantitative Concept]
   861 C0234192:Cold (Cold Sensation) [Physiologic Function]
   827 C1949981:Colds [Pharmacologic Substance]
Meta Mapping (1000):
  1000 C0009443:Common Cold [Disease or Syndrome]
```

- Can e.g. extract CUI from output
- Output can be XML (structured but VERY verbose)

UIMA and Eclipse

- UIMA is NLP pipeline framework
- Eclipse:IDE w/ UIMA integration
  - Installed on CHPC app tree but deprecated
  - Recommend installing your own instance
  - Unless you can't (e.g. need to open HIPAA data)
- Eclipse requires X-Windows server to be running
  - and ssh -Y to forward X calls from CHPC

Other Software at CHPC

- R
  - Not (?) parallelized versions; if you need it or newer versions let me know
- Matlab + many toolboxes / DCS
  - single node 8-core shared-memory parallel
  - 64 proc. distributed memory (embarrassingly parallel only)
- Python
  - 2.x numpy, scipy, matplotlib; 3.x?
- SAS (subject to licensing)

Finally...

- Let us know if you need some other package
  - Factors: cost, hardware/OS requirements, licensing
- Report problems by emailing issues@chpc.utah.edu
- Any questions – contact me!
  - Sean.Igo@utah.edu
  - CHPC Cubicle: Ask at desk in 405 INSCC (president's circle)
  - BMI: 421 Wakara, #225 (near Dr. Chapman's office)

Questions?

Parallelizing Your Task

- Most packages I've shown are single-processor!
  - Dedicated parallel software would be nice...
  - Can write your own, not always practical
- Different ways to run existing sw on parallel clusters
- Many tasks are “embarrassingly parallel”
  - i.e., capable of being decomposed into sub-problems that do not depend on one another
  - e.g., parsing several text files; can just send 1/**n** of the files to parsers running on **n** processors

Parallelizing Your Task

- Embarrassingly Parallel is nothing to be ashamed of!
- However, dividing tasks naively may not give each processor the same amount of work
- That is, 1/**n** of the documents/sentences/etc. may not be 1/**n** of the work
- Initial tests with MetaMap show that dividing over documents is a terrible way to use it

Parallelizing Your Task

- Slightly better: “deal” tasks to processors as they become available
  - with fine granularity should be very efficient
- Other things to consider:
  - Per-invocation overhead
  - Integrating results
- I'm creating scripts to wrap / distribute software calls (command lines)
  - Talk to me if you need something like this

Default Login Scripts

- CHPC maintains default login scripts that set up environment, now updated to work in protected environment
  - www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.tcshrc
  - www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.bashrc
- Copy to your home directory as .tcshrc or .bashrc
  - This is being done on new accounts
- Can comment out setups for packages not used
- Currently NLP/ML packages not included
- Can customize by creating .aliases file that is sourced at end of the CHPC script

Location of Software

- Currently we place most installations at:
  - /uufs/chpc.utah.edu/sys/pkg
    - Accessible on clusters and some desktops
    - all NLP / ML software is here
- Protected environment also uses the chpc.utah.edu tree
- That is for linux only; Windows / Mac interactive nodes have software installed natively