**Sequential Learning for Materials Science   
  
Citrine Informatics**  
  
Intuition driven

Domain specific machine learning

Uncertainty quantification

jacknife after bootstrap

**Sequential learning framework**

Perform random initial set of experiments to create data set  
 → train machine learning mode  
 → evaluate model with uncertainty estimates over all candidates   
 → choose next candidate based on selection strategy   
 → perform experiment   
 → does test candidate meet specifications?   
  
Maximum uncertainty   
Maximum expected improvement   
Maximum likelihood of Improvement P(f(x) > m) ~ erf[ f(x) – m / sigma(x) ]   
 – takes into account uncertainty of predictions   
  
Inputs : 20-60 features based on composition and processing

Materials Resource Registry   
Materials Data Curation System   
Schema Repository and Registry   
HTE Resource Registry and Repository

Globus – data transfer grid