Knowledge and solutions
for a changing world

Be boundless

Advancing data-intensive
discovery in all fields

Data Science Methods for Clean Energy Research (DSMCER)

UW DIRECT
(Data Intensive Research Enabling Cutting-edge Tech)
https://uwdirect.github.io

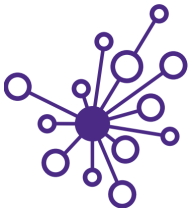
David A. C. Beck (dacb)
chemical sciences & eScience Institute

Who is that guy Dave?

- Computer Science, BS
- Biomolecular Structure & Design / Medicinal Chemistry, PhD
  - Scalable parallel software for molecular sims
- Director of Research, eScience Institute
  - Manage data science research programs
- Research Associate Professor, ChemE
  - Software and Data Science methods at the intersection of chemistry, biology, energy, health & environment

Not open source! ☹

What is this class about?



- Survey of Data Science methods
  - Tool selection
  - Best practices
  - Not about designing new algorithms
- Group project using these methods
- Life changing

I need more details!

- Class website:
  - https://uwdirect.github.io
    - Let's go there now!

- Logistical items
  - Laptops – bring 'em!
  - Slack – use it!
  - Software – install it!

I need more details!

- We will talk more about the structure of the two courses this afternoon

- Questions now?

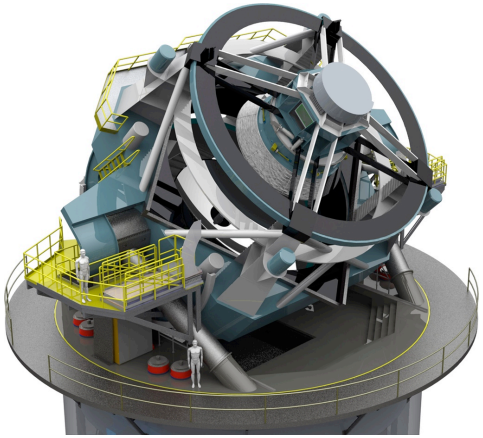
What's this all about?

- Data

- Science & engineering
  - Chemical sciences
  - Science & engineering at large
    - Environment, energy, health, urban

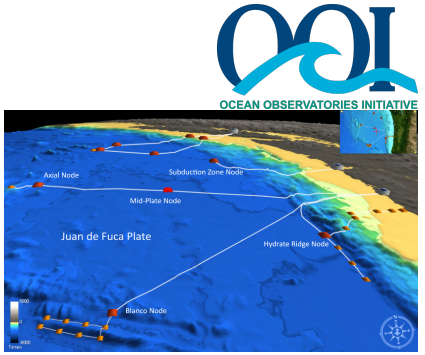
OMG, so much data!

- All fields of science: “data poor” → “data rich”

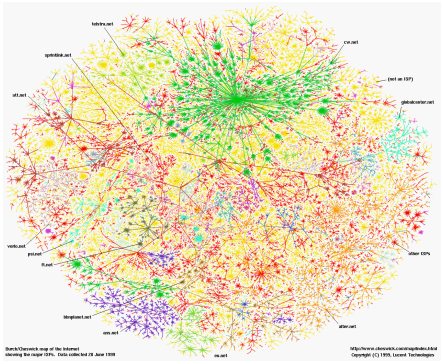


Astronomy: LSST

Physics: LHC



Oceanography: OOI



Sociology: Social networks

Biology: Sequencing

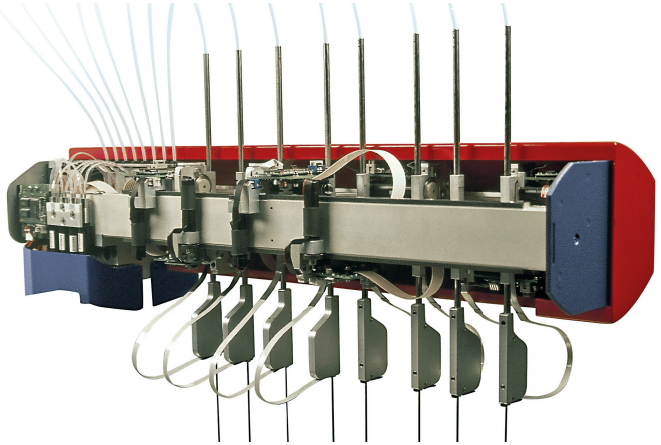
Economics: POS terminals

Neuroscience: EEG, fMRI

On the origins of data

- Chemical sciences is not an exception
  - Robotic high-throughput instrumentation
    - E.g. Parallel high-throughput solution phase synthesis for combinatorial chemistry and characterization

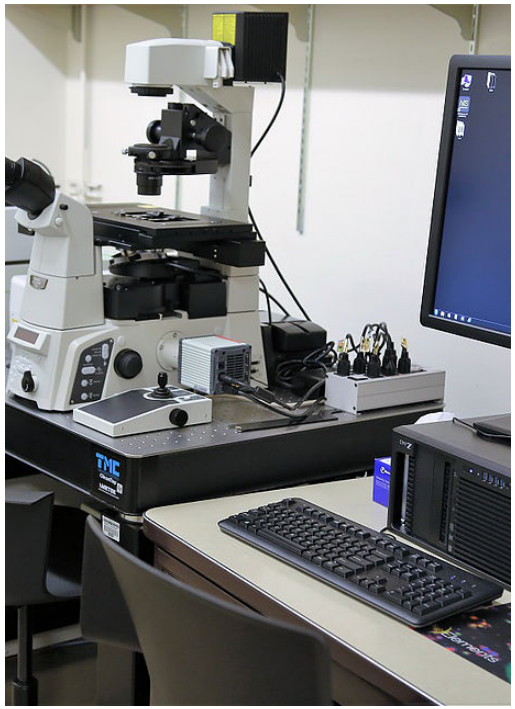
Tecan Xantus



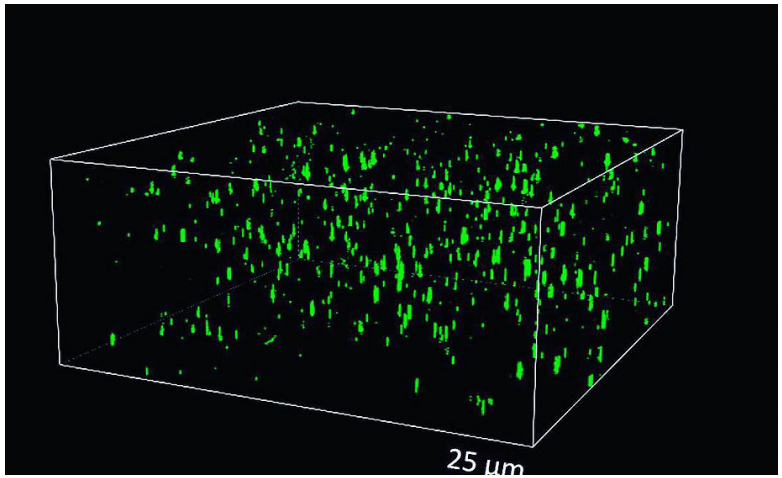
Modular plug and play arms &
GUI for experiment configuration

On the origins of data

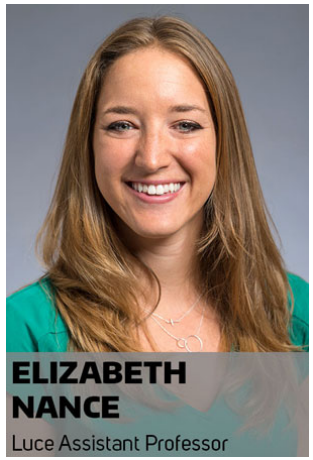
- Chemical sciences is not an exception
  - High resolution imaging for particle tracking & 3D reconstruction



http://www.nancelab.com

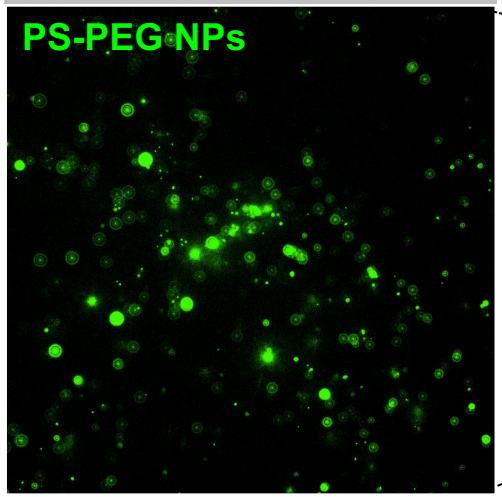


Understanding nanoparticle behavior in physiological environments with implications for therapeutic delivery

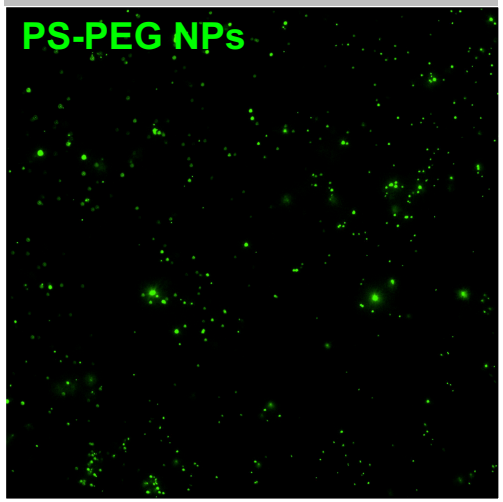


On the origins of data

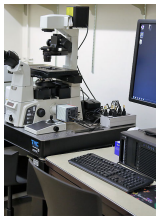
Cortex



"Mid" brain



Not just static images!



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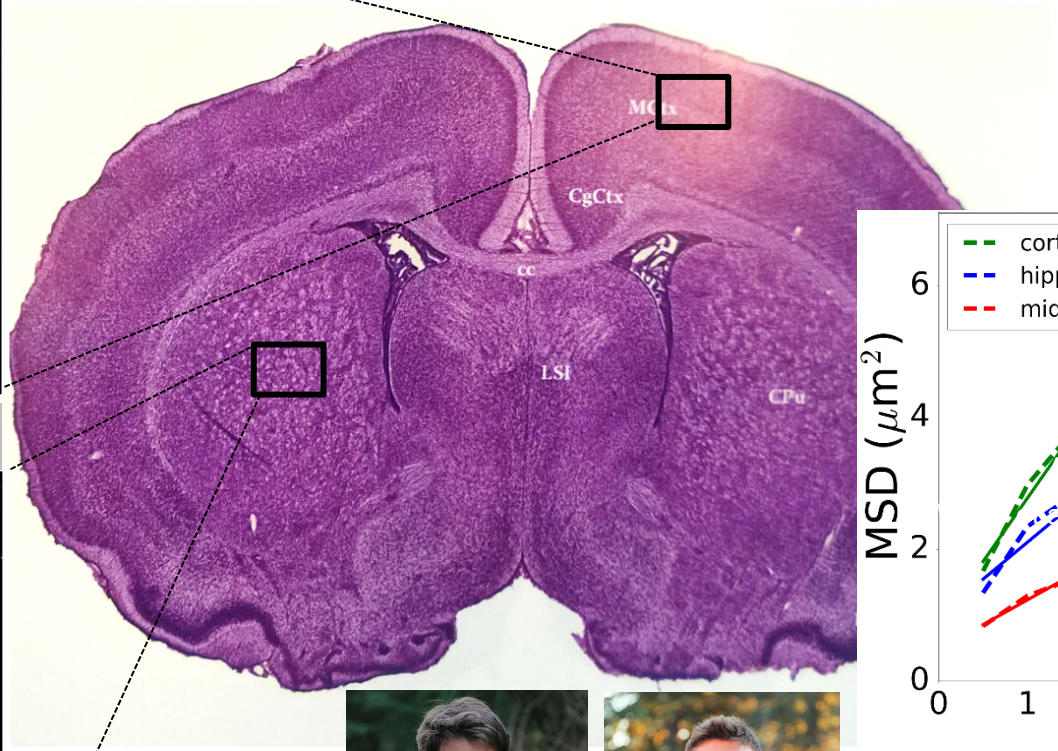
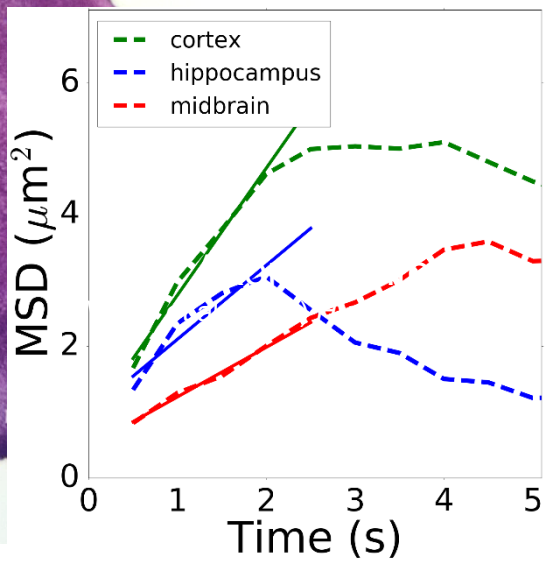




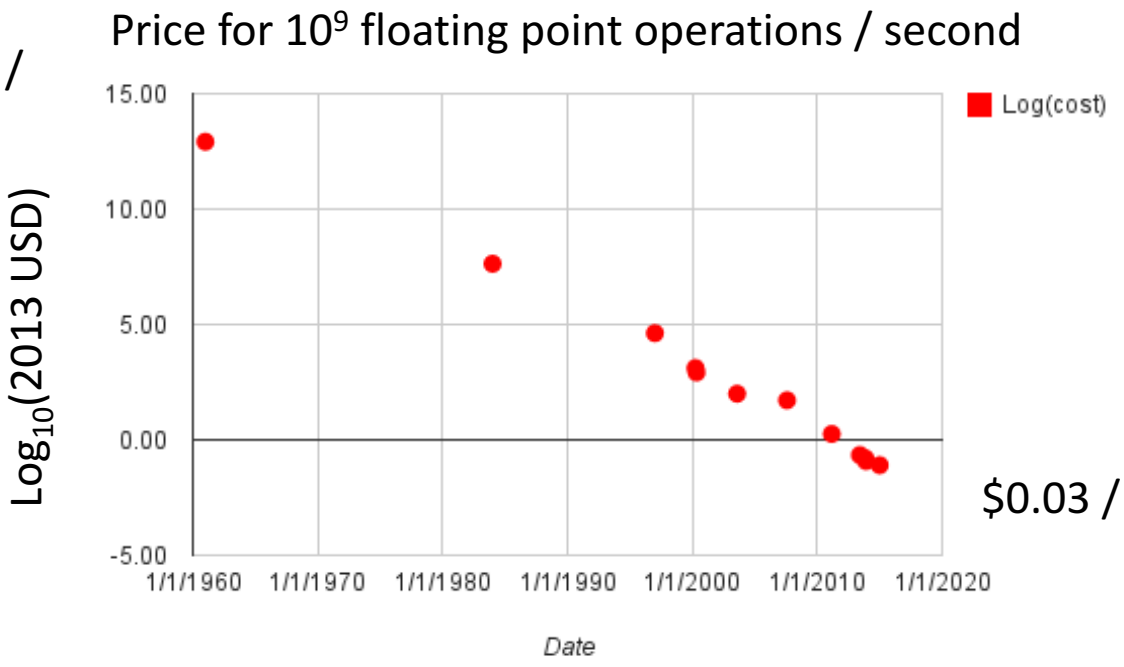
Chad Curtis

Mike McKenna

On the origins of data

- Chemical sciences is not an exception
  - Exponential decline in computing cost

$145 billion / gigaflop in 1964



$0.03 / gigaflop in 2017

https://aiimpacts.org/trends-in-the-cost-of-computing/

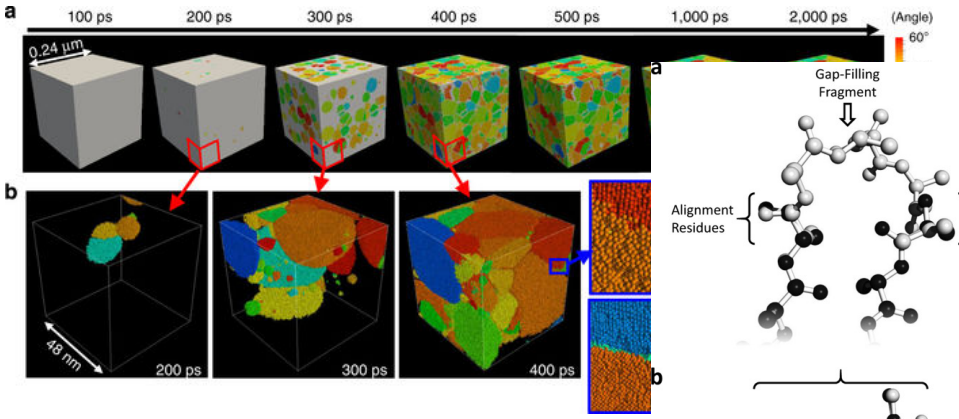
On the origins of data

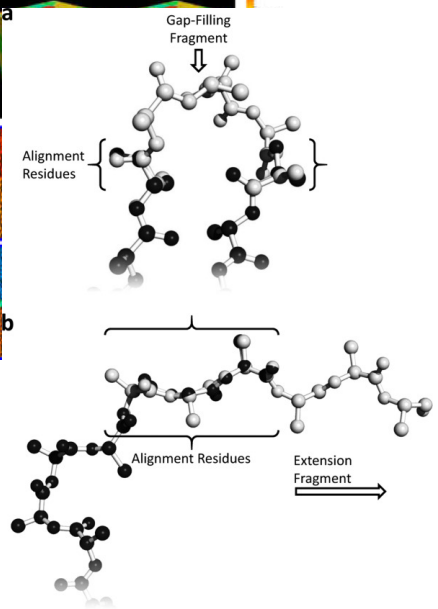
- chemical sciences is not an exception
  - Substantial decline in storage cost

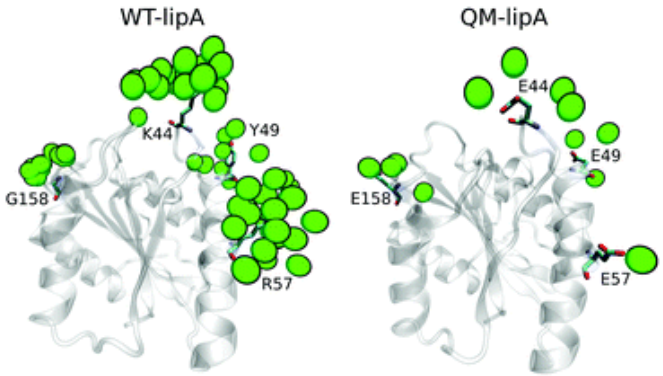
Average cost per gigabyte

On the origins of data

- Chemical sciences is not an exception
  - Cheaper faster compute and storage resources
    - E.g. bigger[1], more[2], longer[3] molecular simulations







1.Shibuta, *et al*. *Biophys. J.* 2017
2. Rysavy, *et al. Prot. Sci*. 2014.
3. Sprenger, *et al*. *Roy. Soc. Chem.* 2017.

On the origins of data

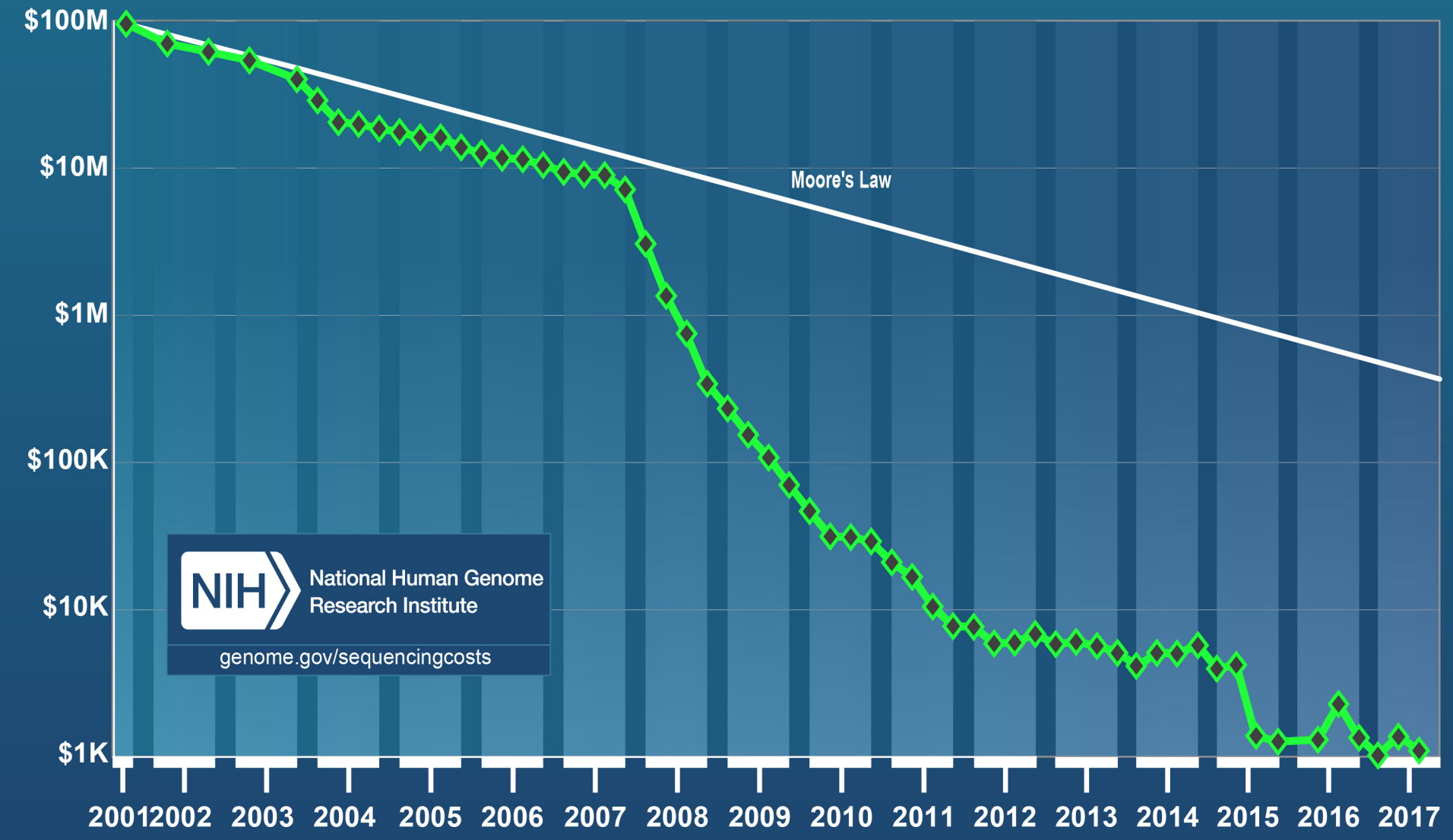
- Chemical sciences is not an exception
  - Synthetic and systems biology
    - E.g. high throughput gene sequencers[1], long read gene sequencers[2], ultra-cheap gene sequencers[3]

1. Illumina HiSeq
10^{10} bases / day

2. PacBio Sequel
10^{9} bases / day

3. Oxford Nanopore MinION
~$1000 USB powered

Cost per Genome



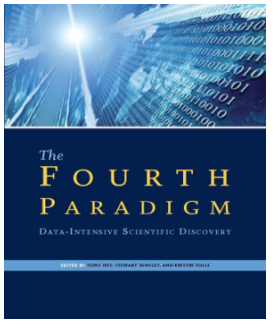
On the origins of data

- chemical sciences is not an exception
  - Industrial sensor networks & internet of things (IoT)
    - E.g. EU's public-private partnership RECOBA (BASF led)

- Massive coordinated sensor networks with high volume data streams
- Online model predictive control
- Process optimization and cost reduction

Evolution of discovery

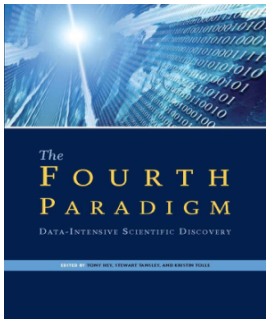
- Paradigm shifts in discovery
  - Empirical & experimental



2009, MS

Evolution of discovery

- Paradigm shifts in discovery
  - Empirical & experimental



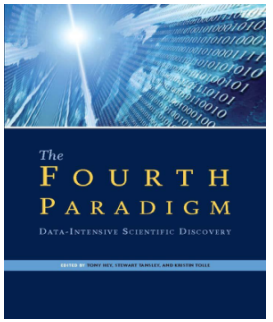
2009, MS

Dave w/ out
Van de Graff

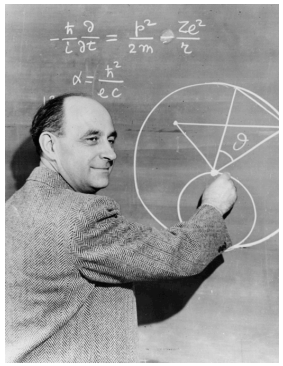
Dave w/
Van de Graff

Evolution of discovery

- Paradigm shifts in discovery
  - Empirical & experimental
  - Theoretical
  - Computational
  - Data-intensive



2009, MS



What makes this possible?

- What the new paradigm of data-intensive discovery and innovation?
  - Deep domain knowledge
  - Data Science
    - Data management
      - Databases, scalable data handling, data curation
    - Machine learning
      - Regression & classification
      - Supervised & unsupervised
    - Statistics
    - Visualization
    - Software engineering

Molecular Data Scientist
Knows thermodynamics **and** machine learning

Data management

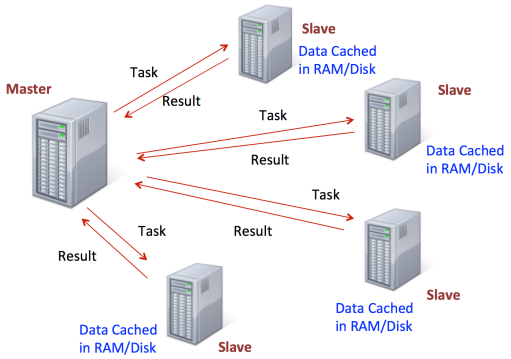
- Data management
  - You've got lots of data, how do you manage it?
    - Not about lab notebooks anymore!
  - Databases
    - Structure and store large, heterogeneous data
    - Slice, subset, and retrieve it efficiently
    - Track provenance and metadata of your data
    - Relational databases
    - Structured Query Language (SQL)

```
SELECT experiment FROM experiments WHERE
experimenter = "Dave 'No Lab Skills' Beck";
```

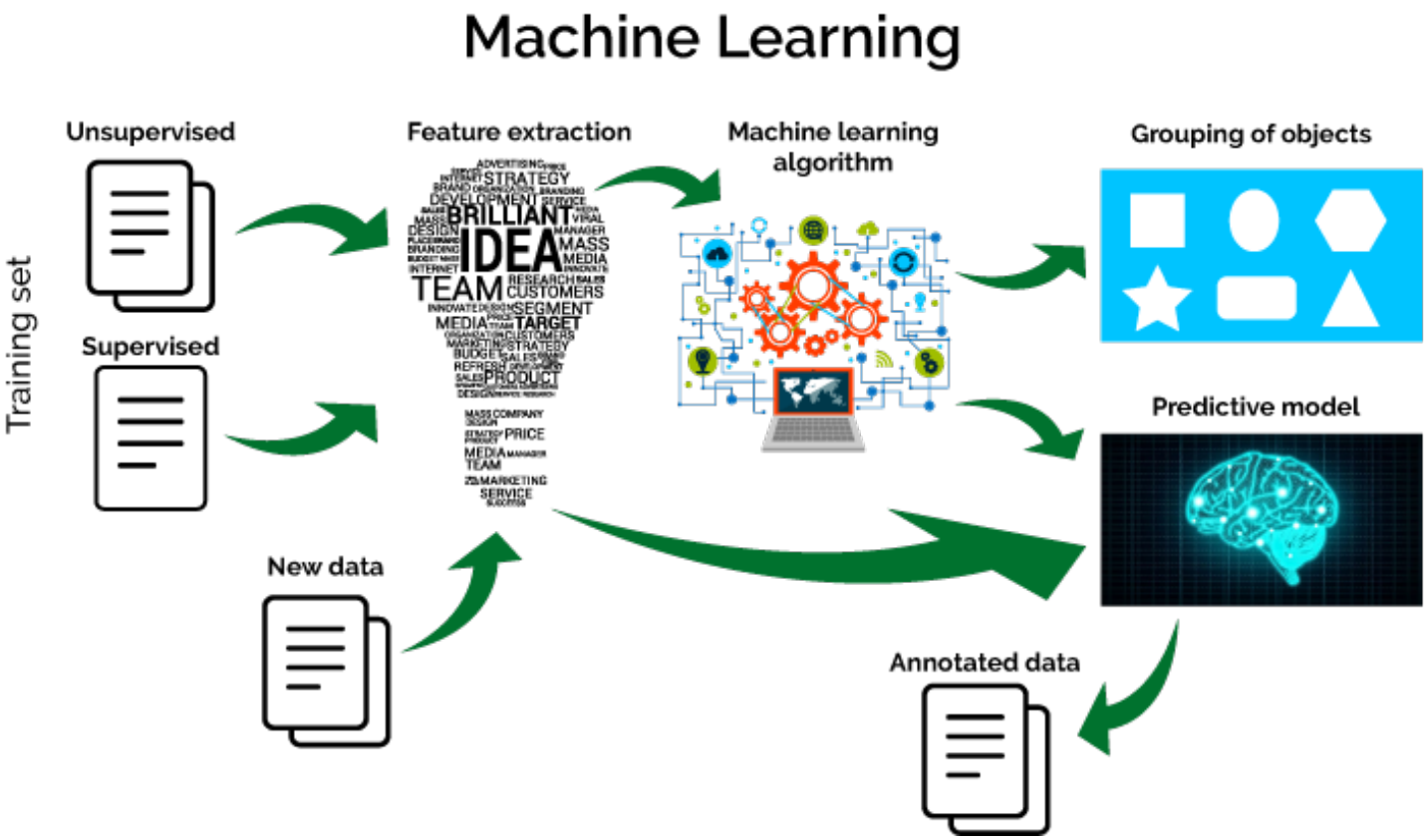
Data management

- Data management
  - Scalable data processing systems
    - Hadoop & MapReduce
    - Apache Spark
      - SQL libraries
      - Machine learning libraries
    - Distribute your data and workload over lots of machines
    - Fault tolerance, scalability

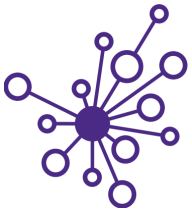
40,000 + nodes (Hadoop)
8,000 + nodes (Spark)



Machine learning



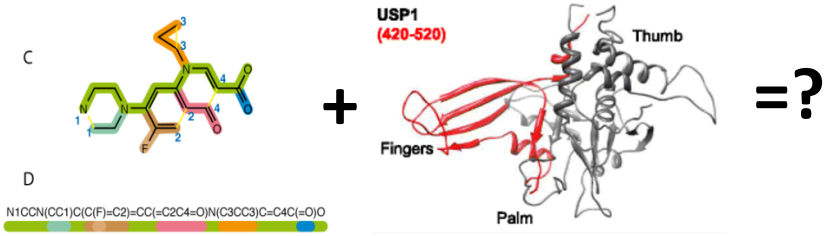
Machine learning



- Regression
  - Predict a numerical response from input features

Machine learning

- Regression
  - E.g. predict binding affinity of small molecules to cancer drug target



Database of 400,000 drug like molecules

Experimental inhibition activities against cancer drug target

Build a regression model that relates molecular features to a numerical measure of inhibition, dissociation constant (Kd)

For a new small molecule, predict the Kd?[1,2]

1. https://github.com/BeckResearchLab/USP-inhibition
2. https://github.com/BeckResearchLab/small-molecule-design-toolkit

Pearl Philip & Rahul Avadhoot

Machine learning

- Regression
  - Predict molecular property or activity from molecular structure

Quantitative Structure Property Relationship (QSPR)

Quantitative Structure Activity Relationship (QSAR)

https://github.com/BeckResearchLab/small-molecule-design-toolkit

Machine learning

- Regression

Features or predictors — Outcome

Molecule	Diffusion (nm/s)	Molecular Weight	C=C bonds	H-bond donors	H-bond acceptors	Kd (fM)
1	8	66	1	0	0	1
2	5	44	2	1	0	12
3	6	95	0	2	0	14
4	7	63	4	0	0	1
5	8	65	1	0	1	4
6	3	91	1	1	1	3
7	6	94	2	0	1	2
8	3	96	1	2	1	2
9	7	57	3	1	1	6
10	6	121	1	0	0	8

Machine learning

- Regression

Features or predictors — Outcome

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8	3	96	1	2	1	2
9	7	57	3	1	1	6
10	6	121	1	0	0	8
11	4	98	2	1	1	????????

New!

Machine learning

- Regression
  - Linear regression

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j .$$

  - LASSO regression (least absolute shrinkage and selection operator)
    - Variable selection (which features are actually useful)
    - Regularization (avoid overfitting to your training data)

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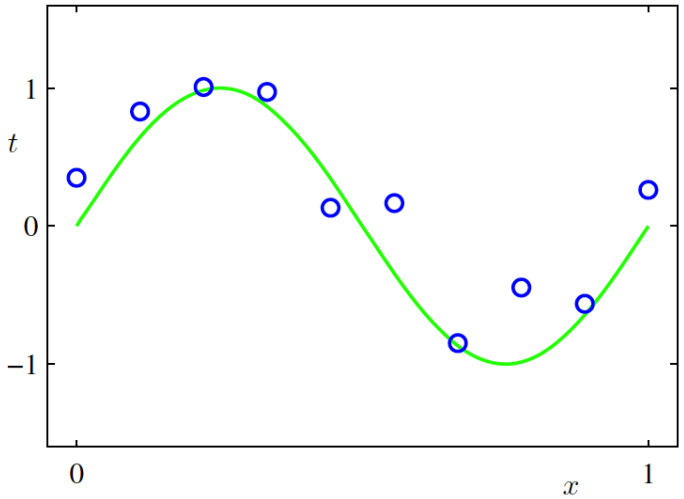
Machine learning

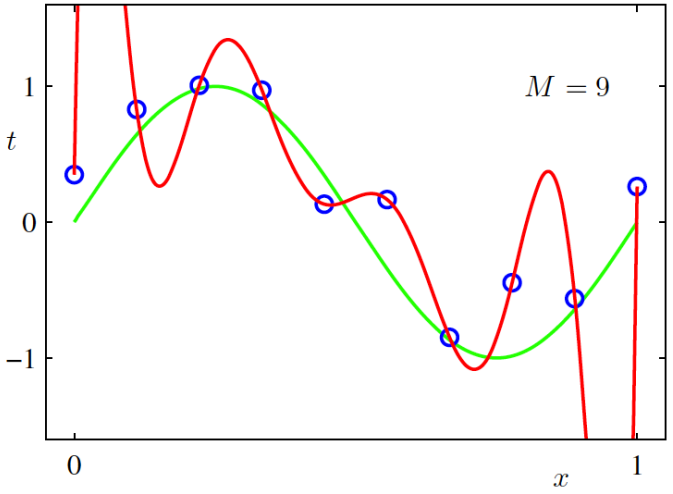
- Overfitting

  "With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."

  - John von Neumann



Points generated from **green** function $f(x) = \sin(2\pi x)$ + noise

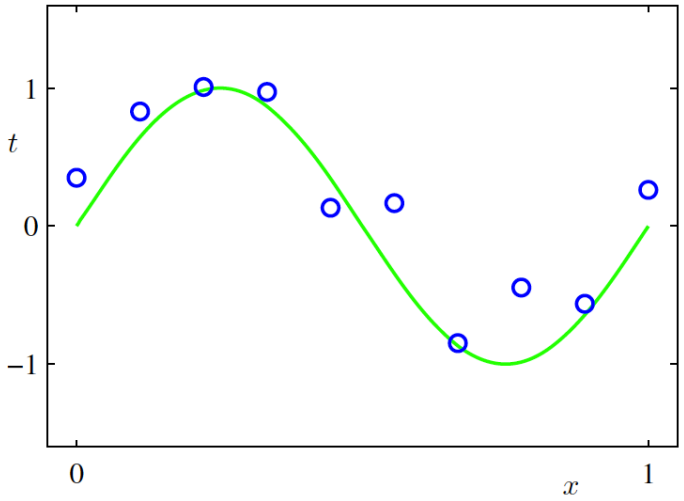


Fitting to points with a polynomial with order $M = 9$

Pattern Recognition and Machine Learning. Bishop, 2006.

Machine learning

- Overfitting
  - Making your model too specific to training data
  - Performs poorly on new data relative to ”truth”



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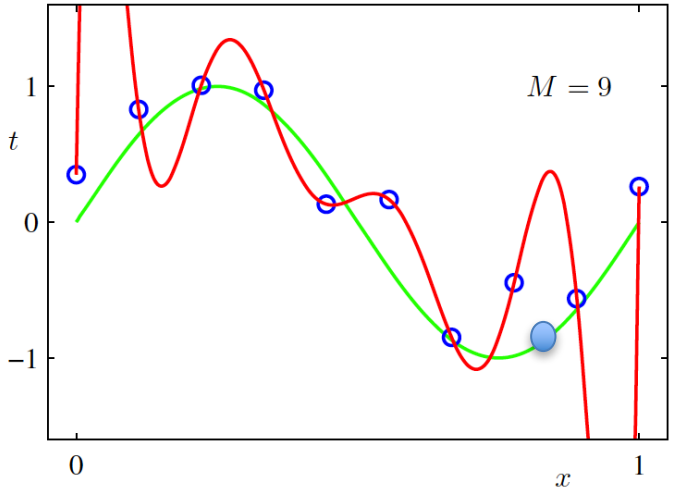
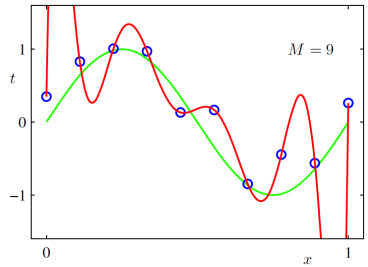


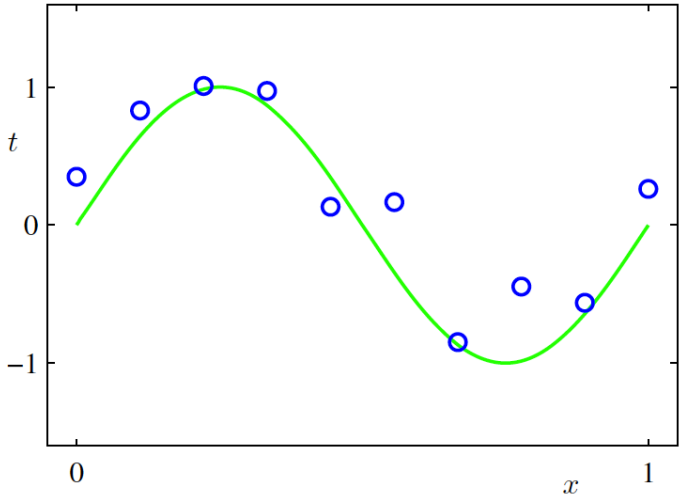
Fitting to points with a polynomial with order $M = 9$

Pattern Recognition and Machine Learning. Bishop, 2006.

Machine learning

- Proper fitting
  - Still fits the training data
  - Performs better on new data





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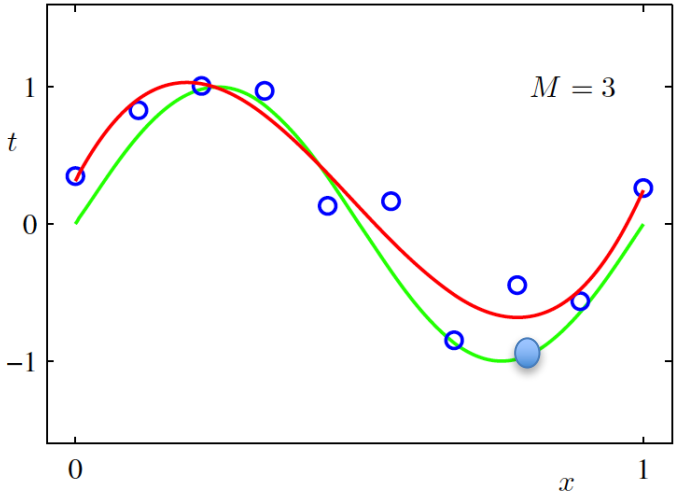
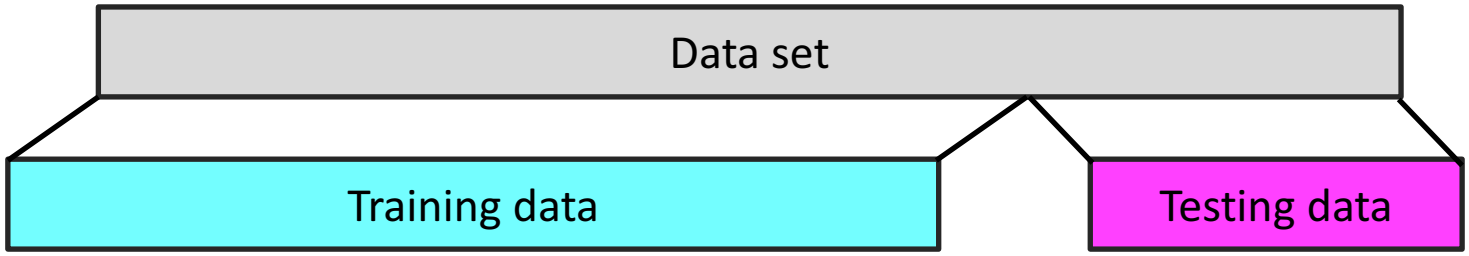


Fitting to points with a polynomial with order $M = 3$

Pattern Recognition and Machine Learning. Bishop, 2006.

Machine learning

- Train / test split
  - How can you identify overfitting?
  - Partition your input data into
    - Training set (e.g. 80%) used to build the ML model
    - Test set (e.g. 20%) used to validate and characterize the error in the model



  - **Never ever ever ever ever** contaminate your model training with data from the test set

Machine learning

- Regression
  - Linear regression

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j .$$

  - LASSO regression (least absolute shrinkage and selection operator)
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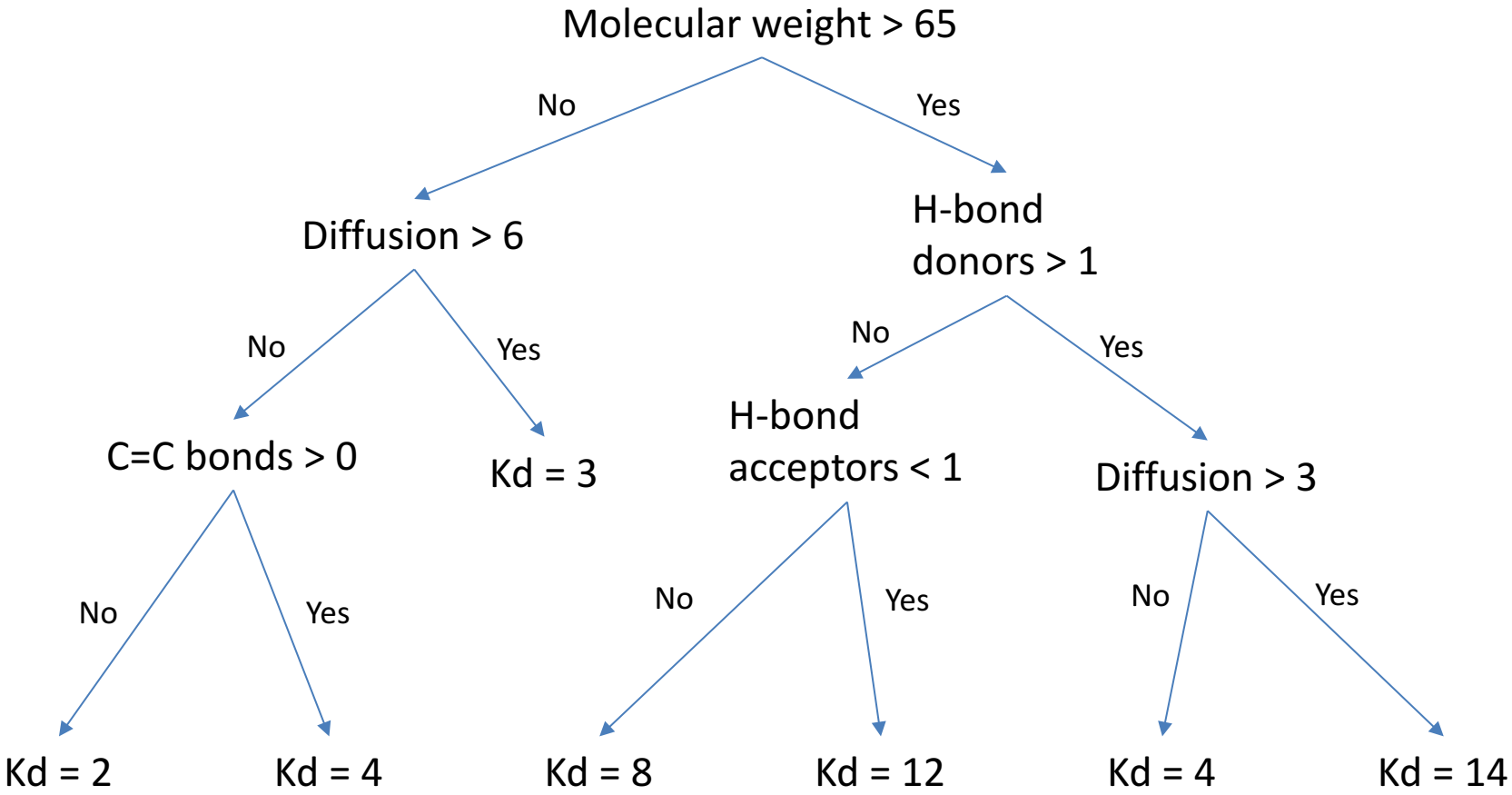
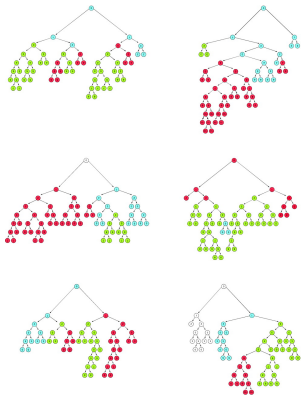
Machine learning

- Regression
  - Decision trees



Machine learning

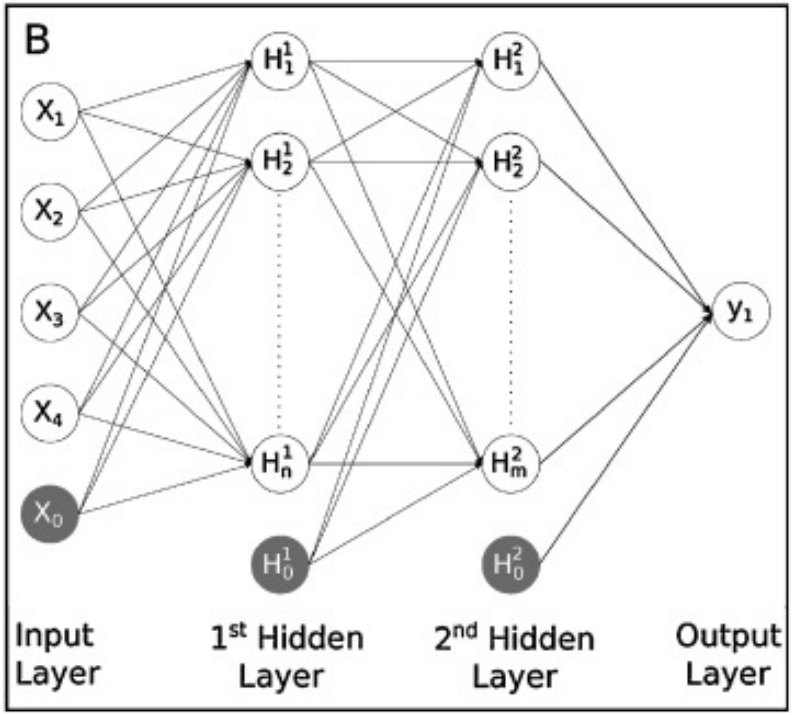
- Regression
  - Multiple trees can describe the data equally well
  - A single deep tree can overfit to training data
  - Ensemble learning
    - Combining several weak learners to get a strong learner
  - Random forests (lots of different decisions trees)
    - Predicted value is mean or mode or median

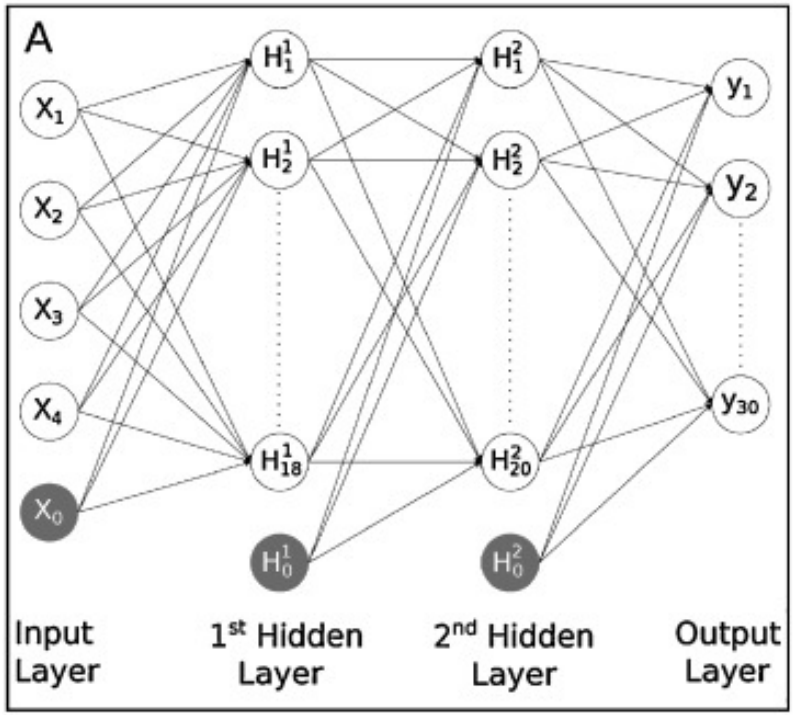


Machine learning

- Regression
  - Artificial neural networks

$y=f(x)$

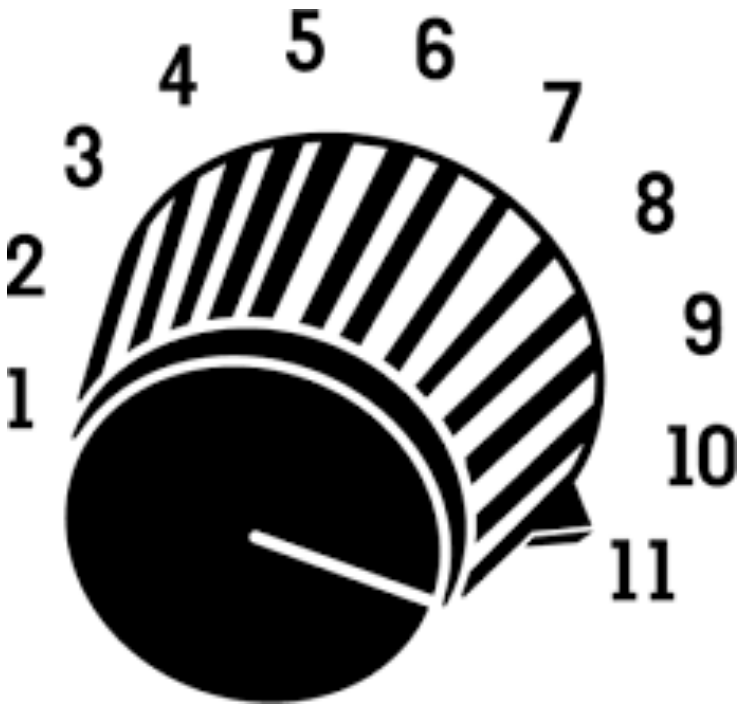




Hough, *et al*. Comp. in Chem. Eng. 2017

Machine learning

- Regression
  - Artificial neural networks

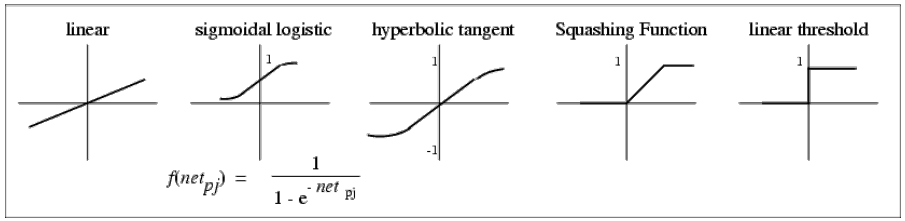


Nodes connect to successive layers via weighted transfer or activation function

Learning occurs by tuning weights (*w*) and parameters of transfer functions

Lots of parameters in neural networks:

- Number of layers
- Number of nodes in each layer
- Transfer function of each layer



Machine learning

- Regression
  - Artificial neural networks
    - E.g. Reducing solution time for lignocellulosic biomass pyrolysis kinetic model

Original kinetic model had

- Inputs like max pyrolysis T, heating rate, mass fractions of C & H in feedstock
- ~100 chemical species
- ~400 reactions
- 30 real valued outputs, e.g.
  - Yields of light & heavy oil
  - Distribution of C functional groups in heavy oil fraction

Solving complete set of stiff ODEs takes nearly 5 seconds

Hough, *et al*. Comp. in Chem. Eng. 2017

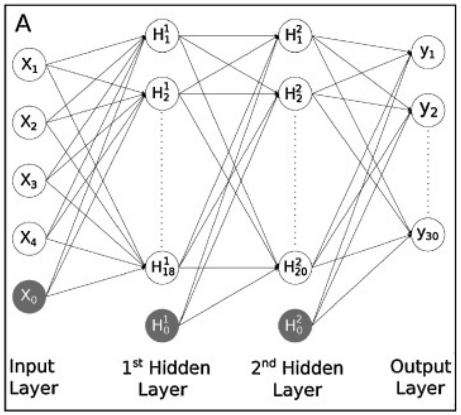
Blake Hough
UW ChemE PhD
Data Scientist,
EnergySavvy

Machine learning

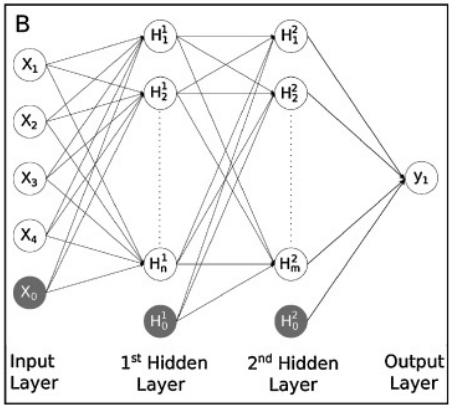
- Regression
  - Artificial neural networks
    - E.g. Reducing solution time for lignocellulosic biomass pyrolysis kinetic model

- Ran the kinetic model 250,000 times varying inputs across their valid range
- Train/test split: 200,000 for training, 50,000 for testing

One model w/ 30 output



30 models w/ 1 output



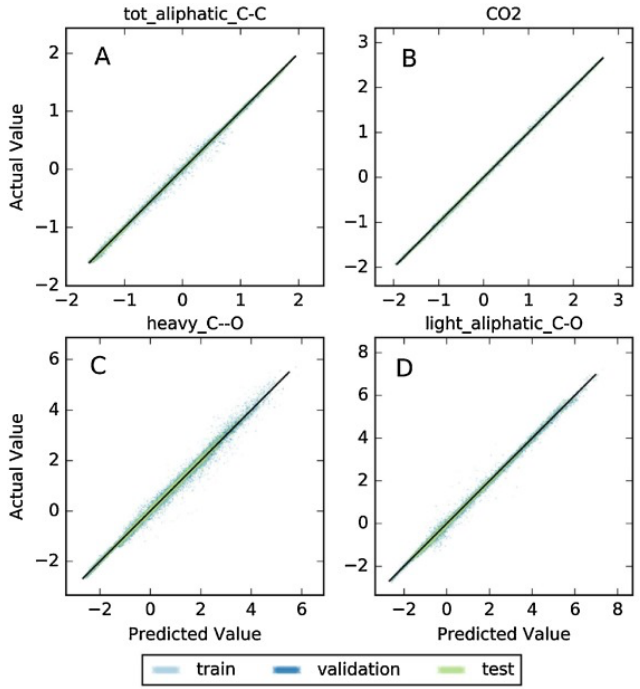
Hough, *et al*. Comp. in Chem. Eng. 2017

Blake Hough
UW ChemE PhD
Data Scientist, EnergySavvy

Machine learning

- Regression
  - Artificial neural networks
    - E.g. Reducing solution time for lignocellulosic biomass pyrolysis kinetic model

$R^2 > .98$ across all outputs



Blake Hough
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Data Scientist, EnergySavvy

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Machine learning

- Regression
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    - E.g. Reducing solution time for lignocellulosic biomass pyrolysis kinetic model

Table 2. Benchmarking results for solving the kinetic model. The time reported is the average of 1000 model calls.

Kinetic model format	Average code execution time (s)
Decision tree	1.106×10^{-4}
Full net	1.690×10^{-4}
Single net	1.747×10^{-4}
30 single nets (run serially)	4.236×10^{-3}
Complete ODE model(B. R. Hough et al., 2016)	4.725

Blake Hough
UW ChemE PhD
Data Scientist,
EnergySavvy

Hough, *et al*. Comp. in Chem. Eng. 2017

Machine learning

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Data Scientist,
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Hough, *et al*. Comp. in Chem. Eng. 2017

Machine learning

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Data Scientist,
EnergySavvy

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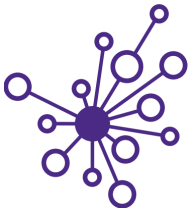
Machine learning



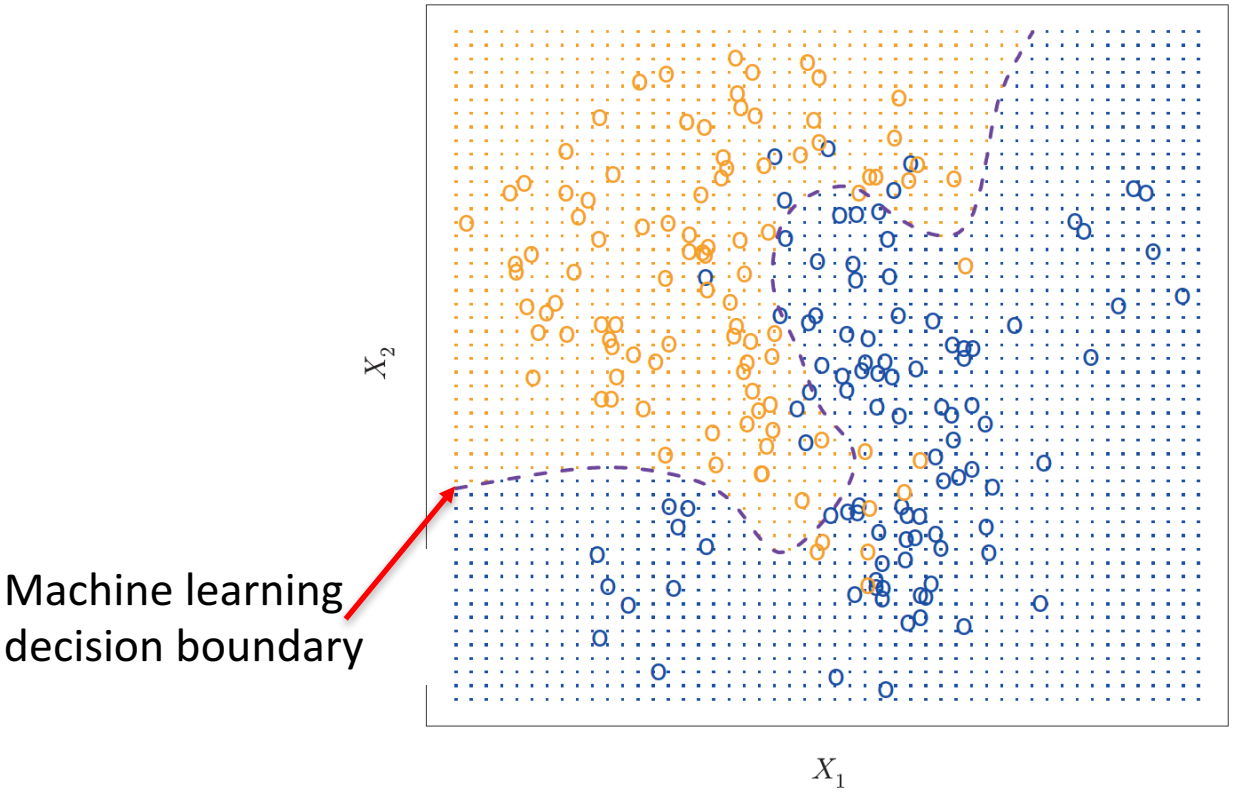
- Regression
  - Artificial neural networks
    - Keras
      - Tensorflow
      - Theano

Machine learning

- Regression
  - Ridge regression
  - Support vector regression
  - ElasticNet
  - Least-angle regression (LARS)
  - Bayesian Regression
  - …
    - An Introduction to Statistical Learning (free PDF)
    - Pattern Recognition and Machine Learning

Machine learning

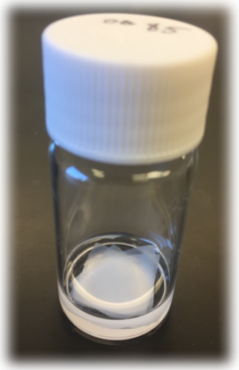
- Classification
  - What state or class does a sample belong to?

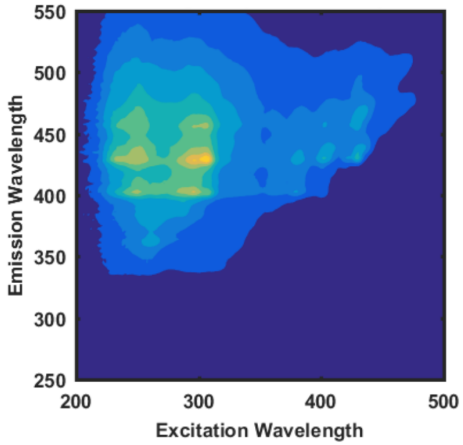


Machine learning

- Classification
  - What state or class does a sample belong to?
    - E.g. Source identification or atmospheric particulate matter (smoke)

- Filter air
- Extract the residue from the filter
- Fluorescent Excitation Emission Spectroscopy (EEM)



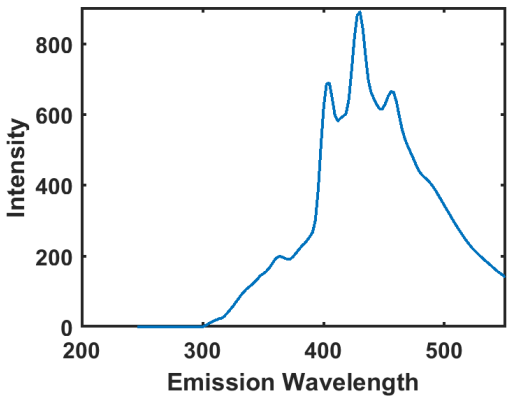


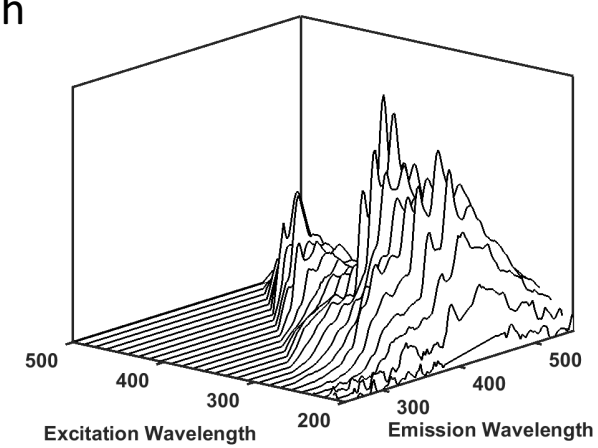
Jay Rutherford
(Posner Lab)

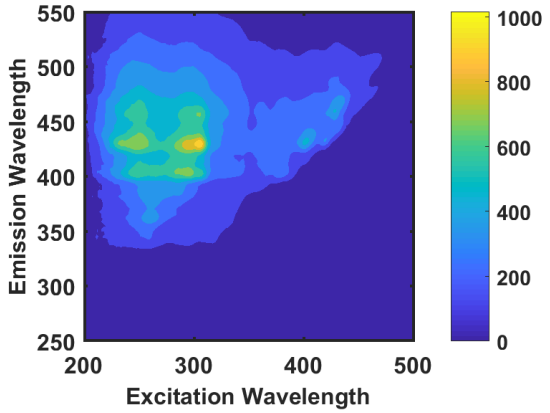
Machine learning

- Fluorescent Excitation Emission Spectroscopy (EEM)
  - Spectra collected at multiple excitation wavelengths
  - Combined into an “Excitation Emission Matrix”

Single excitation wavelength







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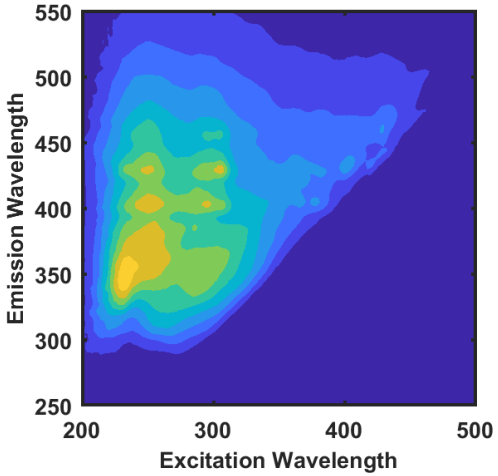
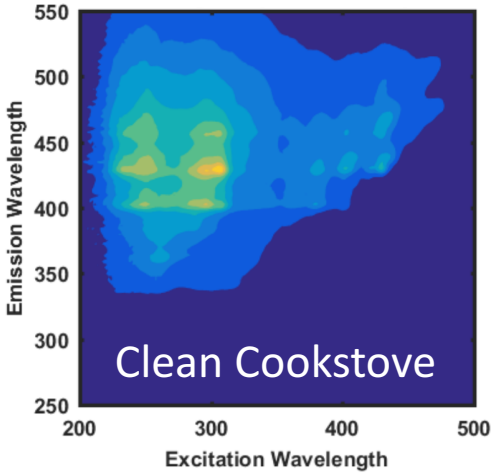
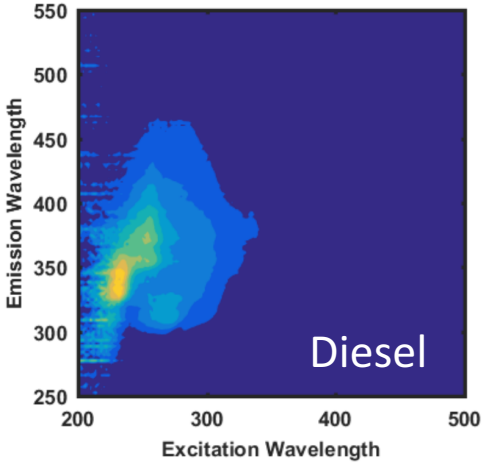
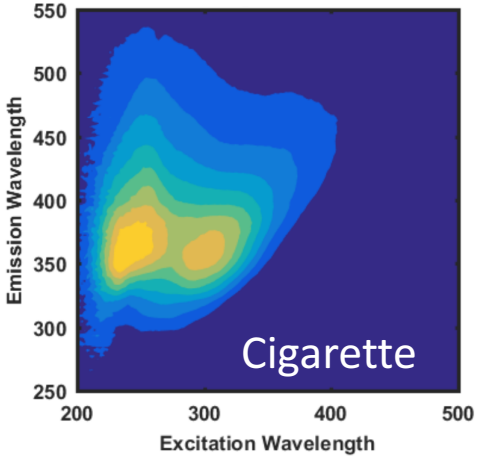
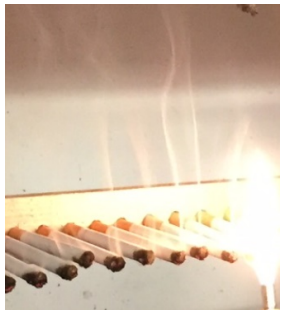


- Classification
  - What state or class does a sample belong to?





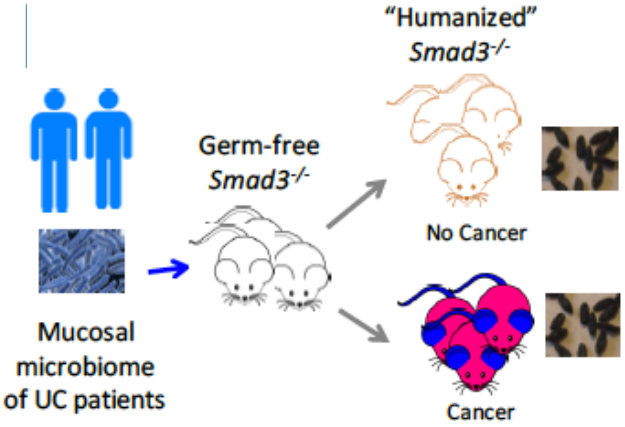




Jay Rutherford
(Posner Lab)

Machine learning

- Classification
  - What state or class does a sample belong to?
    - Ulcerative colitis (UC) & colon cancer diagnostic
      - Take gut microbiome sample from UC patient
      - Inoculate gnotobiotic mice with bacteria
      - See if mice get cancer



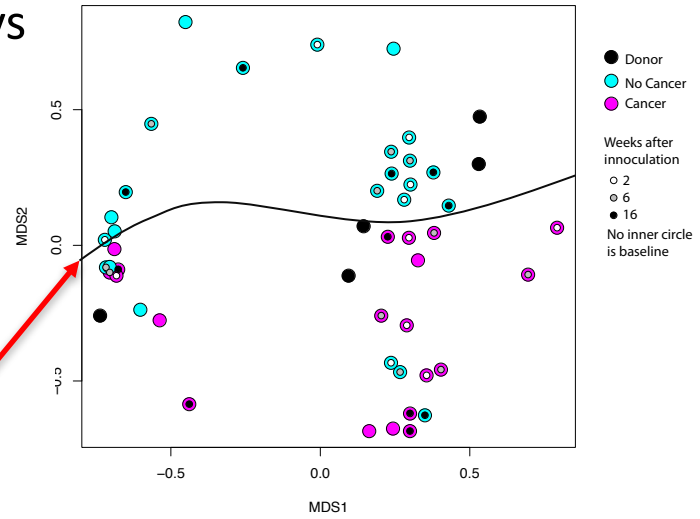
16+ weeks!

Paik, *et al*. Gut Microbes. 2015.

Machine learning

- Classification
  - What state or class does a sample belong to?
    - Rapid ulcerative colitis (UC) & colon cancer
      - Build a model of that relates the gut microbiome structure to cancer likelihood using the gnotobiotic mice data
      - Examine the microbiome of the mucosal sample directly
      - Make cancer assessment in days

Machine learning
decision boundary



Paik, Pershutkina, Meeker, Yi, Dowling, Hsu, Hajjar, Maggio-Price, Beck. Gut Microbes. 2015.

Machine learning

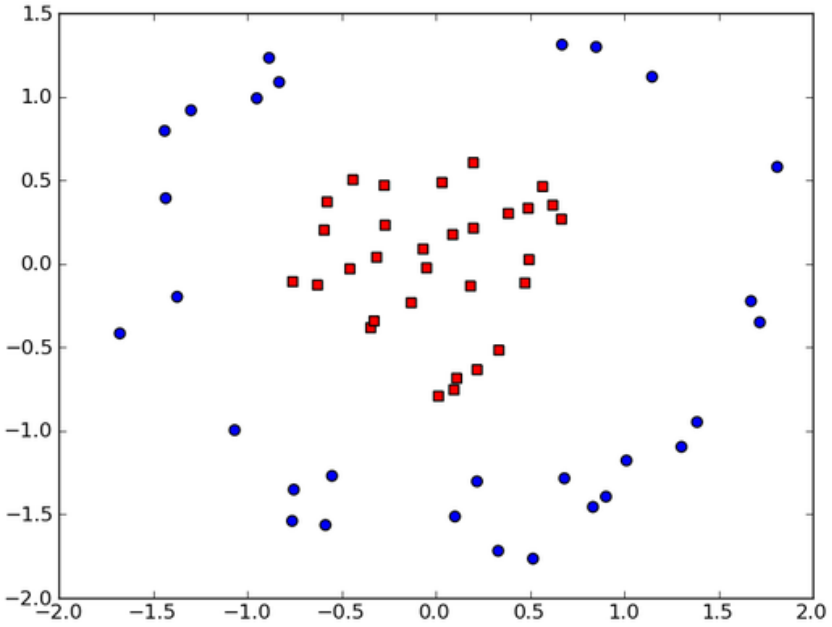
- Classification
  - What state or class does a sample belong to?
    - Rapid ulcerative colitis (UC) & colon cancer

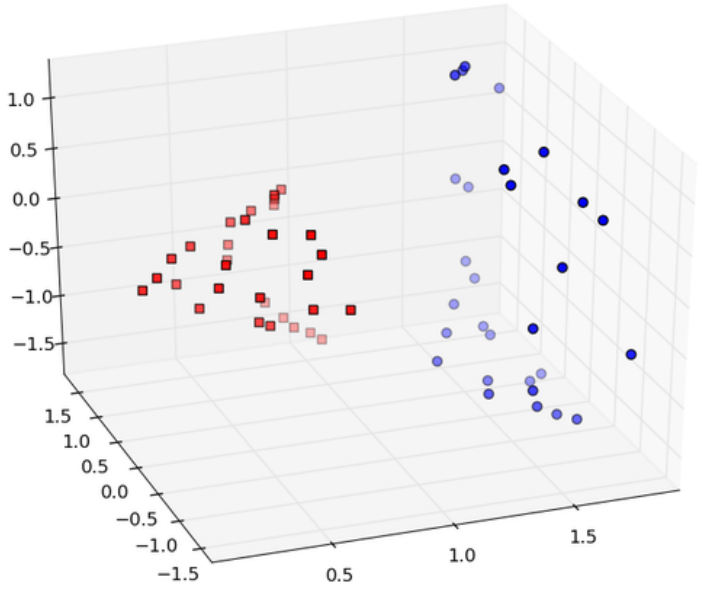
Ultra-rapid, super cheap, metagenome sequencing + Data Science =

Machine learning

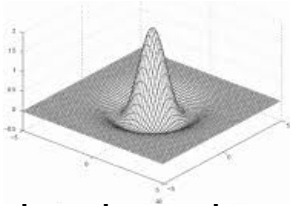
- Classification
  - What state or class does a sample belong to?
  - Methodological approaches:
    - Naïve Bayes Classifier
      - Probabilistic classifier that assumes conditional independence
    - Support vector machines
    - Linear discriminant analysis
    - Neural networks

Machine learning





Original feature space



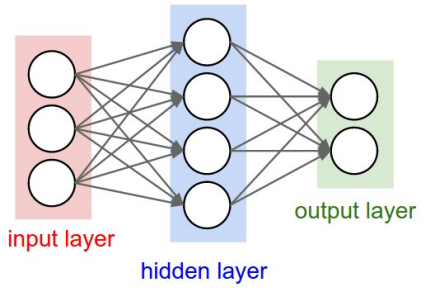
Transformed feature space

Now we can easily find a plane that separates the points!

http://bit.ly/2xOOVZ4

Machine learning

- Classification
  - What state or class does a sample belong to?
  - Methodological approaches:
    - Naïve Bayes Classifier
      - Probabilistic classifier that assumes conditional independence
    - Logistic regression
    - Support vector machines
    - Linear discriminant analysis
    - Neural networks



http://cs231n.github.io/neural-networks-1/

Machine learning

- Classification
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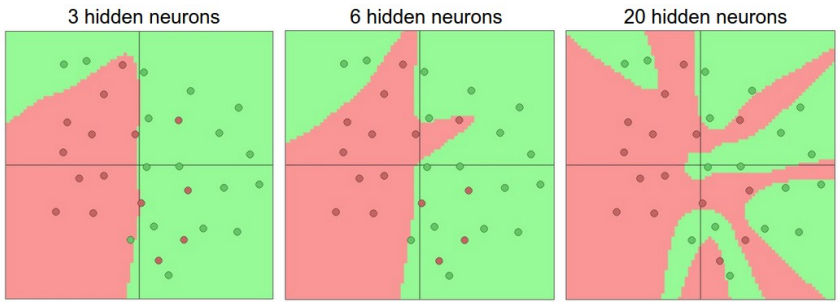


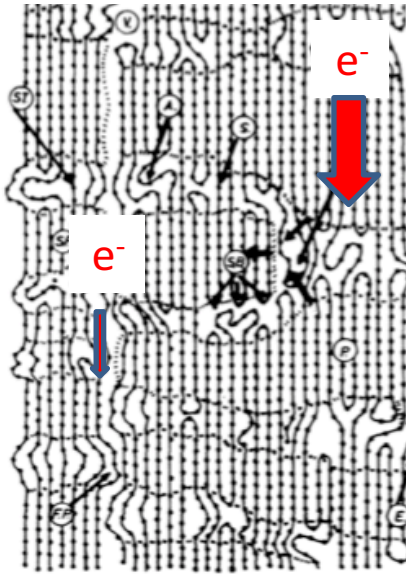
http://cs231n.github.io/neural-networks-1/

Regression + classification

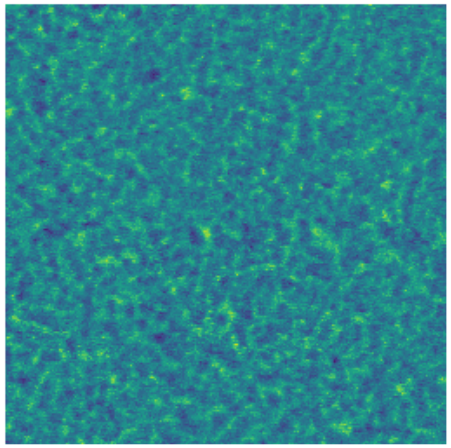
- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

Morphological Analysis of Nanostructured Thin-films (MANA-T)

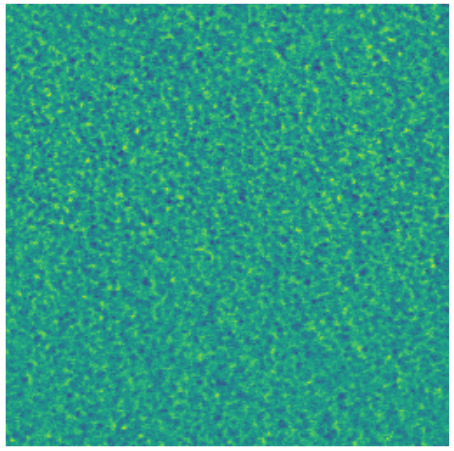
Morphology of Polymer Thin Films



Atomic Force Microscopy



Control



Annealed

DIRECTee

Wes Tatum (Luscombe Lab)

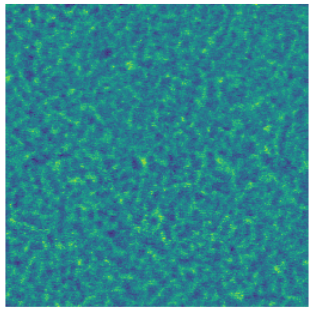
Regression + classification

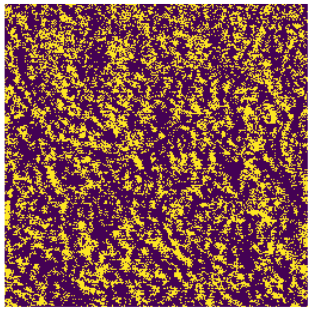
Adhesion PixelClassifier EuclideanClassifier

- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

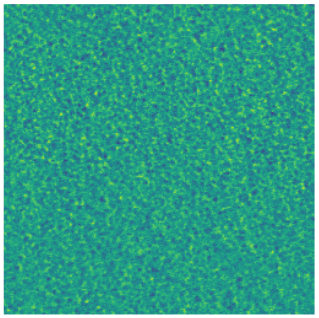
AFM image PixelClassifier

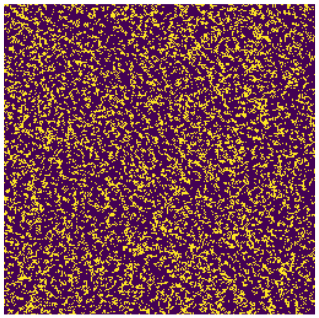
Control Sample





Annealed Sample





Yellow = Crystalline
Purple = Amorphous

DIRECTee

Wes Tatum
(Luscombe Lab)

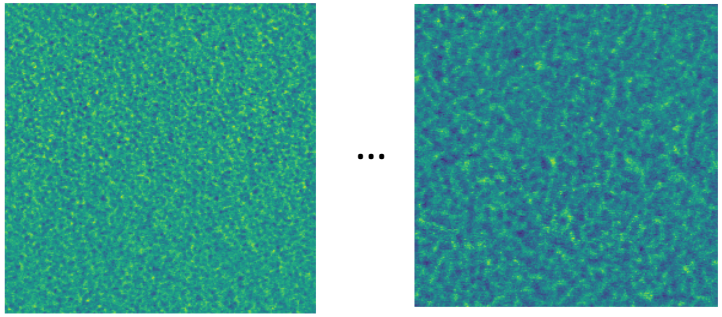
Regression + classification

Adhesion PixelClassifier EuclideanClassifier

- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

Many thin polymer files characterized by AFM

Create a library of images with films with different annealing parameters



1. Build library of data → 2. Classify domains of each AFM scan → 3. Train and validate neural network using library → 4. Use validated neural network to rapidly optimize

DIRECTee

Wes Tatum (Luscombe Lab)

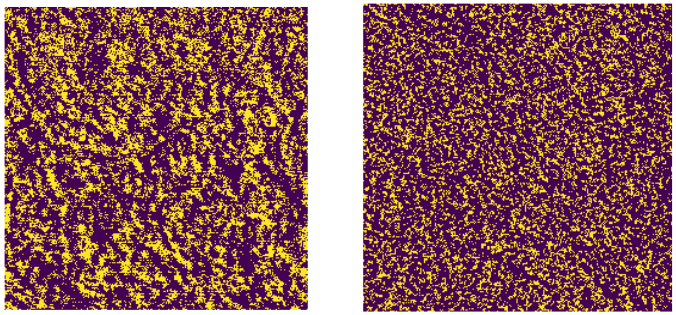
Regression + classification

Adhesion PixelClassifier EuclideanClassifier

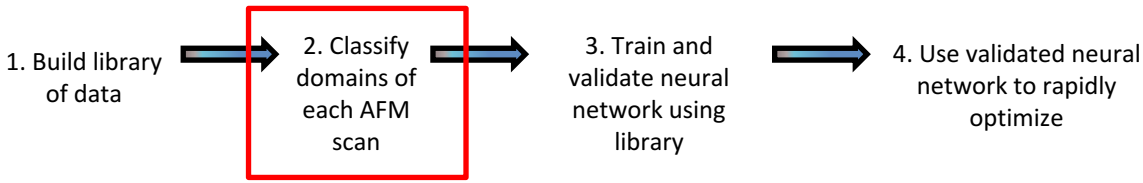
- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

Classify the domains in the images as crystalline or amorphous

For each material can compute ratio



Yellow = Crystalline
Purple = Amorphous



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Wes Tatum
(Luscombe Lab)

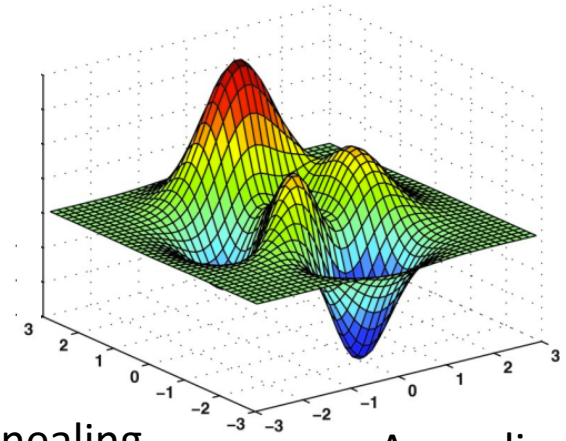
Regression + classification

Adhesion PixelClassifier EuclideanClassifier

- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

Train neural network to predict morphology based on annealing parameters

Fraction classified as amorphous vs. crystalline



1. Build library of data → 2. Classify domains of each AFM scan → **3. Train and validate neural network using library** → 4. Use validated neural network to rapidly optimize

DIRECTee

Wes Tatum (Luscombe Lab)

Regression + classification

Adhesion PixelClassifier EuclideanClassifier

- Sometimes you really need it all
  - E.g. Optimize annealing parameters in creation of polymer thin films

Use the neural network to rapidly optimize the process for idealized functionalization

1. Build library of data → 2. Classify domains of each AFM scan → 3. Train and validate neural network using library → 4. Use validated neural network to rapidly optimize

DIRECTee

Wes Tatum (Luscombe Lab)

Supervised vs. unsupervised

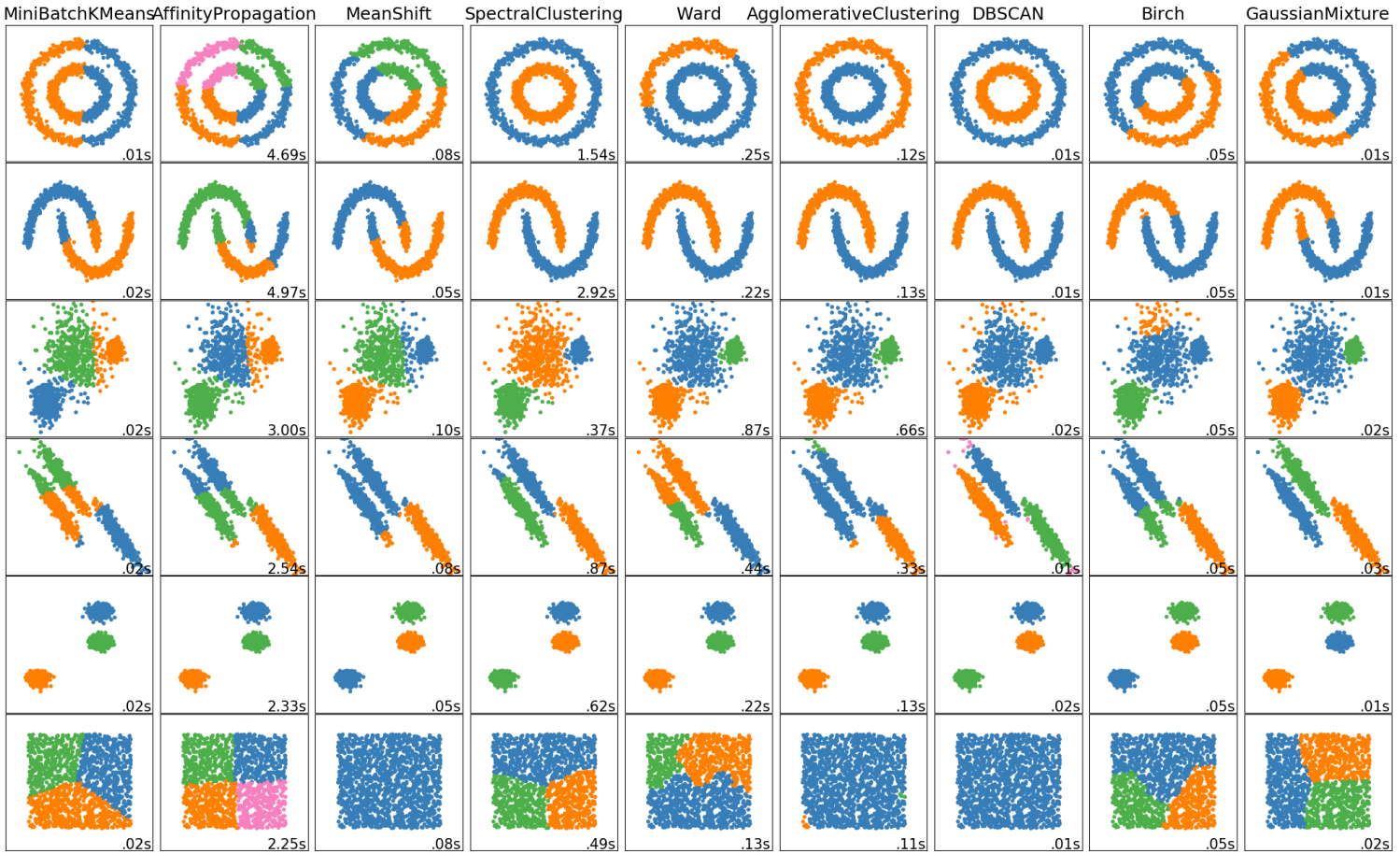
vs.

Supervised vs. unsupervised

- Supervised
  - Input data is ”labeled”
    - Know the Kd
    - Know the source of the atmospheric particulates
- Unsupervised
  - No labels associated with the data
  - Discovering structure in the data

Discovering hidden structure

- Clustering



http://scikit-learn.org/stable/modules/clustering.html

Discovering hidden structure

- Clustering
  - E.g. In an industrially relevant bacterium, identify genes that are co-regulated across conditions

Find all the genes with similar expression profiles (clustering)

Search their upstream regions for regulatory motifs

DIRECTee

Alexey Gilman

Jiayuan Guo

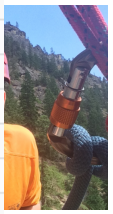
cture

Expression strength of genes in cluster

Predicted regulatory sequences

Location of sequences relative to gene

DIRECTee

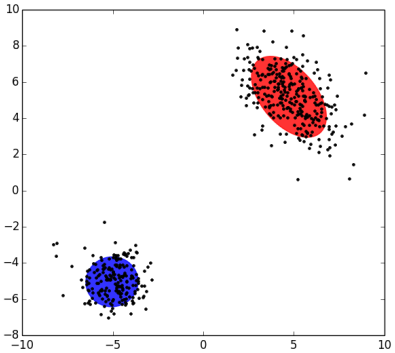


Alexey Gilman

Jiayuan Guo

Discovering hidden structure

- Clustering
  - K-means
    - Find k clusters in the data
  - gdbscan
    - Find clusters with a given local density
  - DPGMM
    - Dirichlet Process Gaussian Mixture Model
    - Grows Gaussians across your data



Visualization

- How can you convey a complex multivariate data set to stakeholders & peers?
  - E.g. how does water order around amino acids?

Run 100ns+ molecular dynamics simulations of G-G-X-G-G where X is each of 20 amino acids

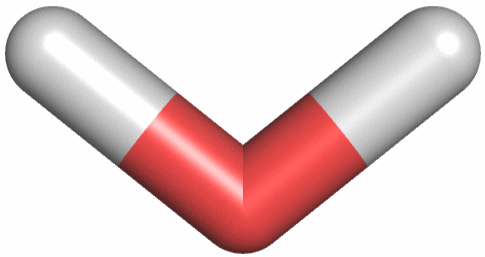
Build a model of the occupancy and orientation at a grid of sites around amino acids

Visualization

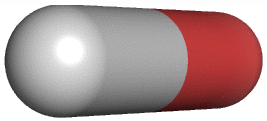
Dynamics

Representation

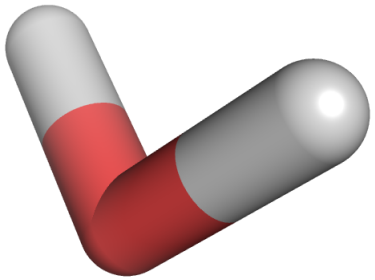
H_2O Ordering

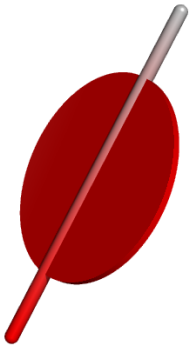


Dipole (length)



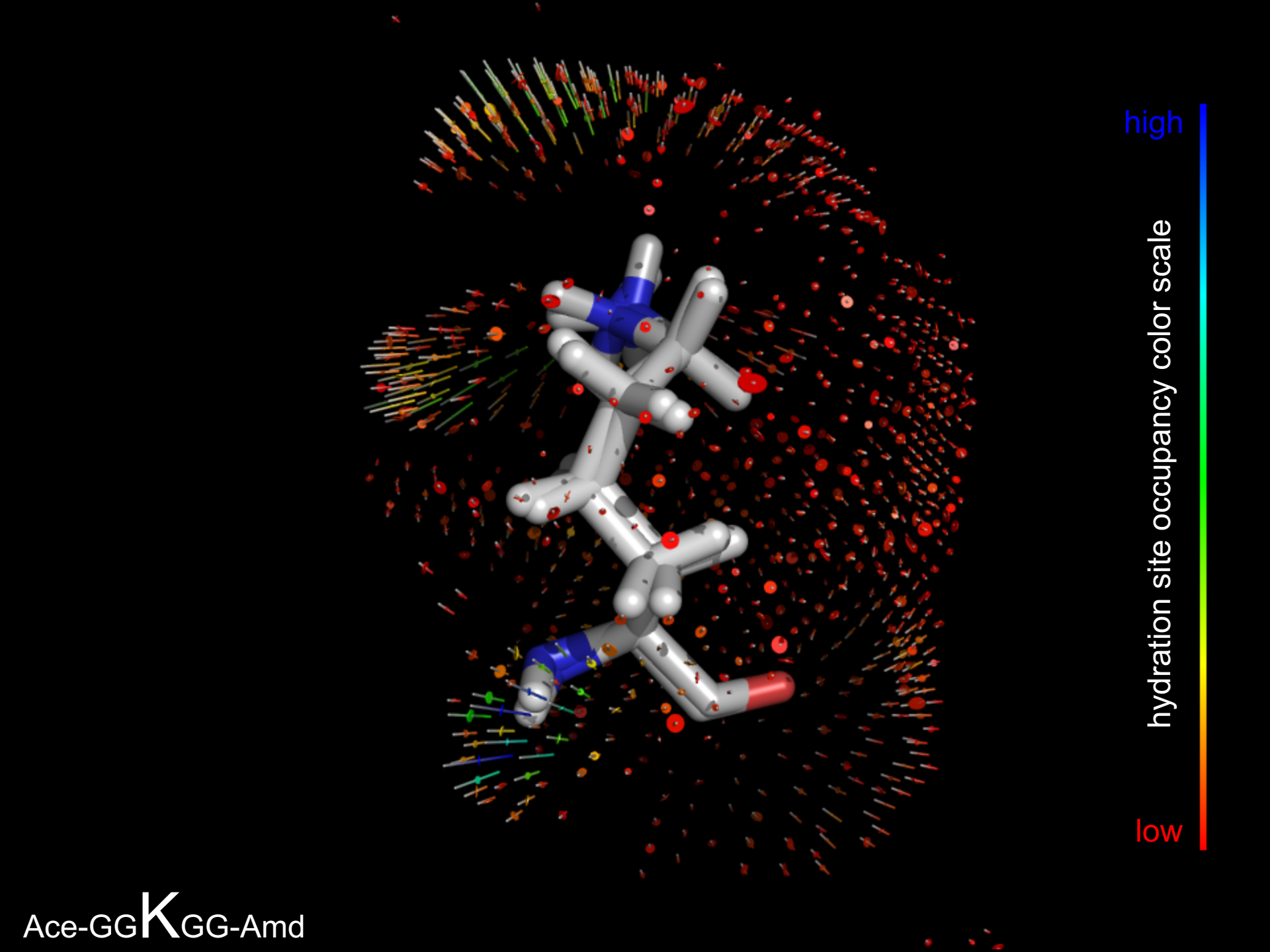
Plane (disc radius)

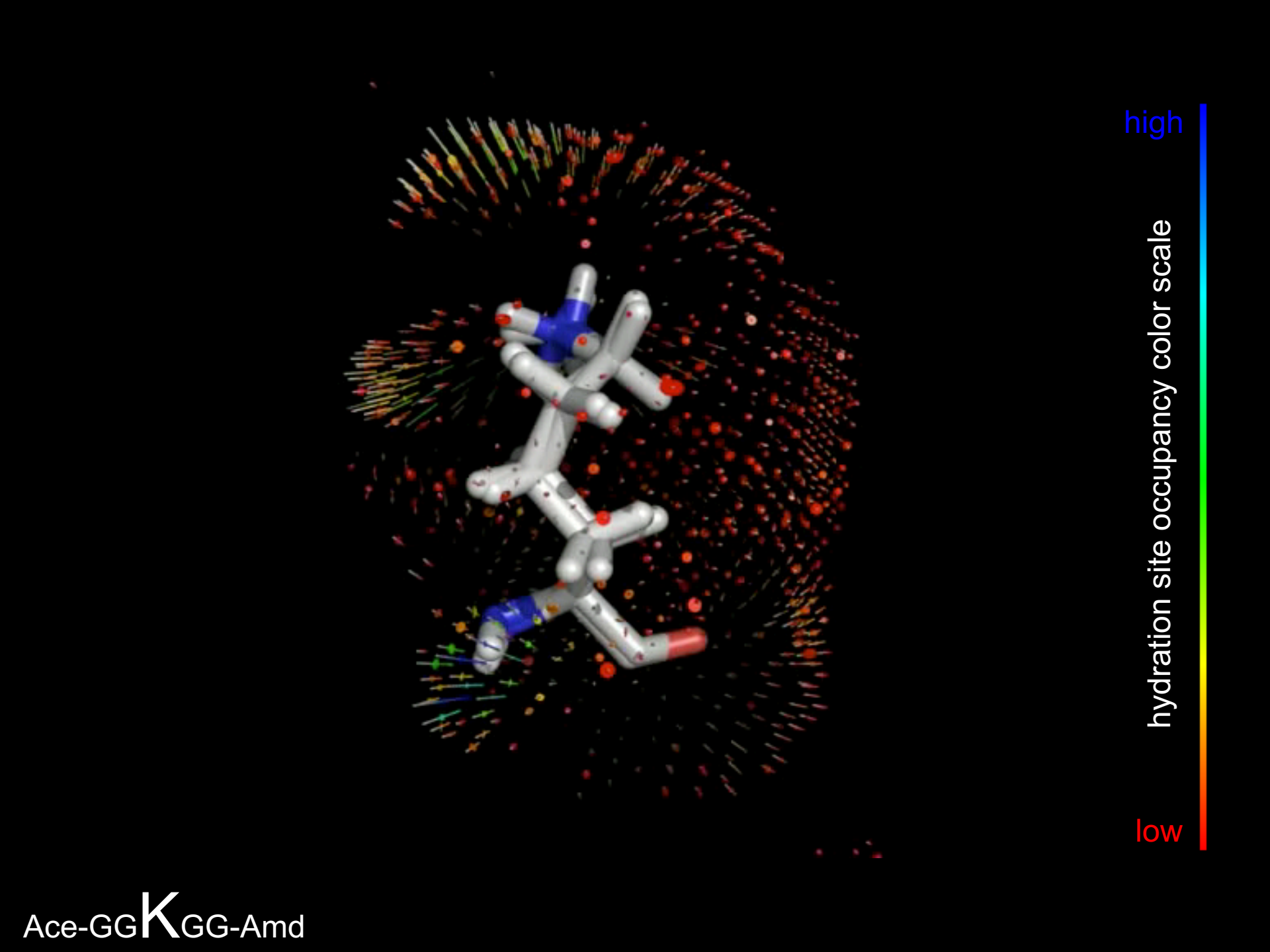


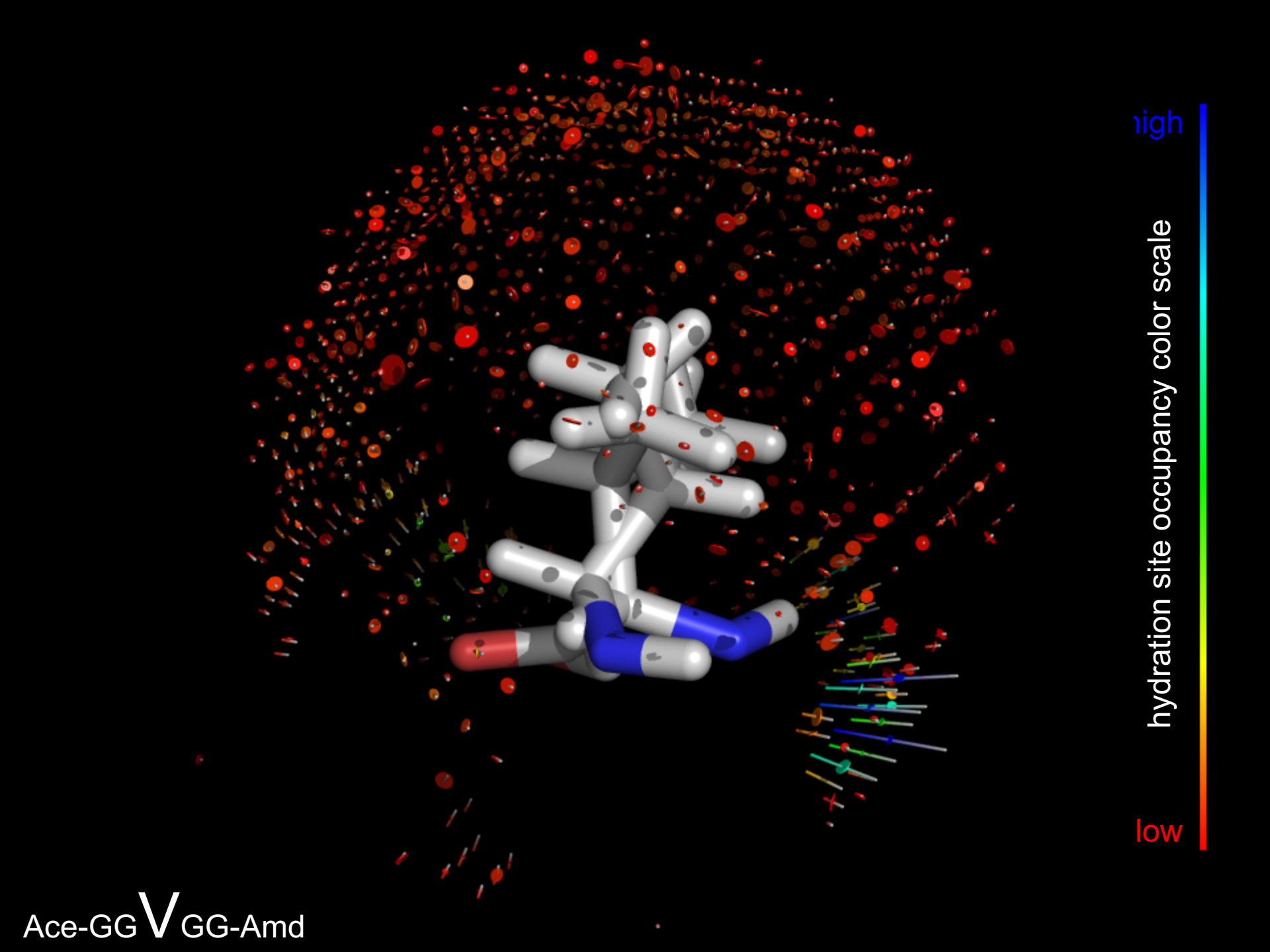


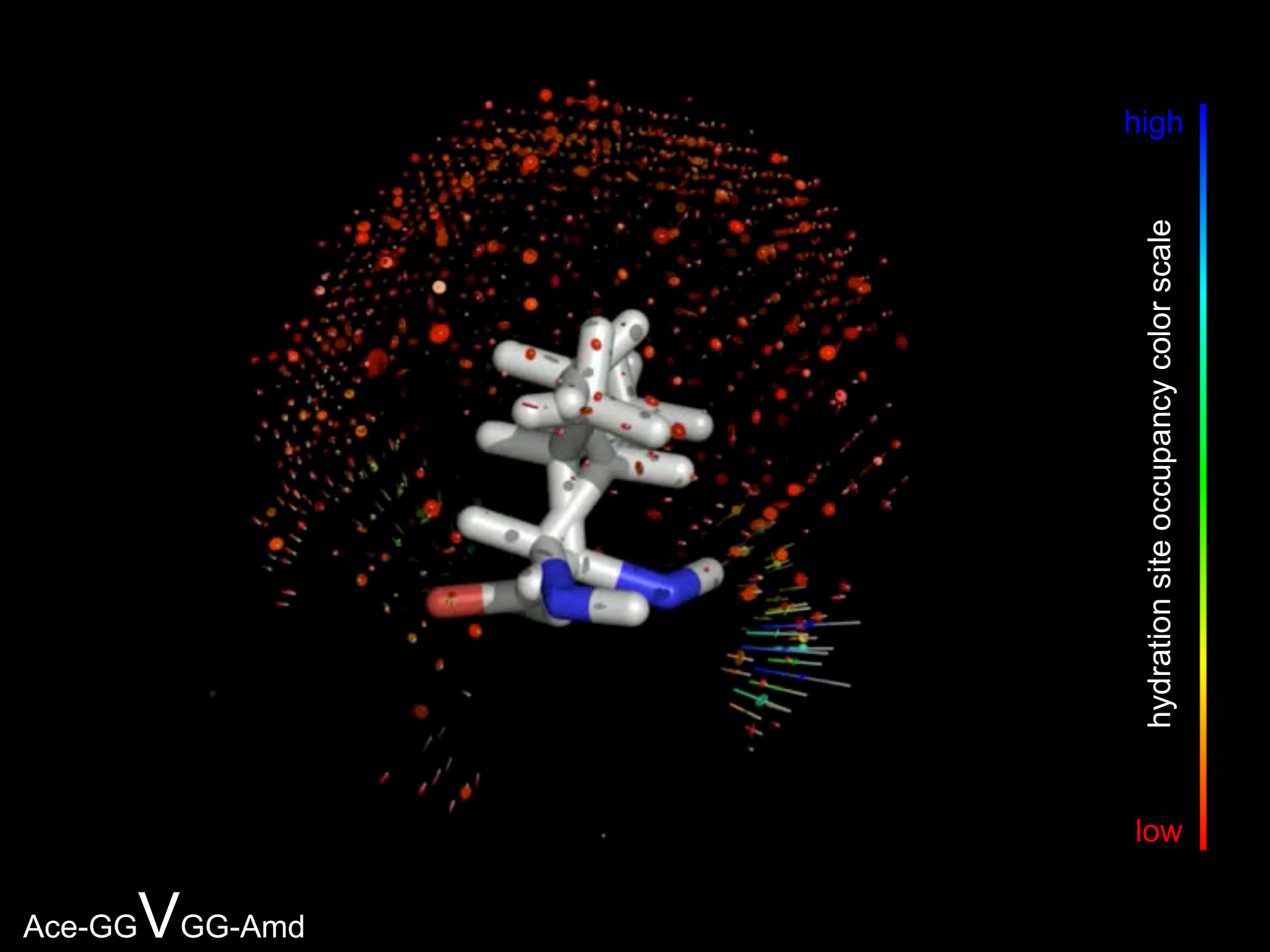
Dipole & Plane

Beck *et al.* Biophys. Chem. 2002.


high
hydration site occupancy color scale
low
Ace-GGKGG-Amd


high
hydration site occupancy color scale
low
Ace-GGKGG-Amd


high
hydration site occupancy color scale
low
Ace-GGVGG-Amd


high
hydration site occupancy color scale
low
Ace-GGVGG-Amd

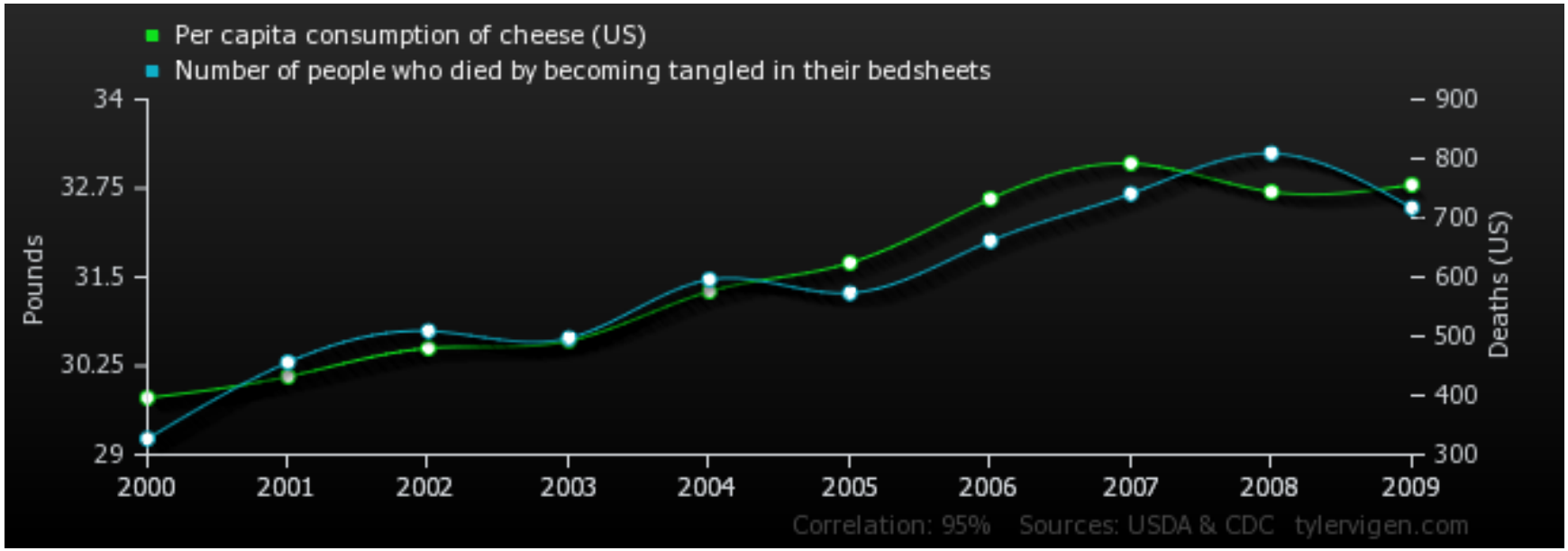
Statistics

- Experimental design
  - Power analysis, sample size, effect size
  - Reproducible results
- Correct statistical test
  - Not everything follows a normal distribution!

William Sealy Gosset
"Student"

Statistics

- Multiple hypothesis testing & *p*-hacking



Correlation: 0.947091

http://tylervigen.com/view_correlation?id=7

Software engineering

- Your code should not look like this:

```
I n t,e,l[80186],*E,m,u,L,a,T,o,r[1<<21],X,*Y,b,Q,R;I
Z*i,M,p,q=3;I*localtime(),f,S,kb,h,W,U,c,g,d,V,A;N,O,P=983040,j[5];SDL_Surface*k;i(F,40[E]=!!o)i(
z,42[E]=!!o)i(D,r[a(I)E[259+4*o]+O])i(w,i[o]+=~(-2*47[E])*~L)i(v,G(N-S&&1&
(40[z((f^=S^N)&16),E]^f>>C-1)))J(){V=61442;$;O--;)V+=40[E+O]<<D(25);}i(H,
(46[u=76,J(),T(V),T(9[i]),T(M),M(P+18,=,4*o+2),R(M,=,r[4*o]),E]=0))s(o){$;O--
;)40[E+O]=1&&1<<D(25)&o;}i(BP,(*i+=262*o*z(F((*E&15)>9|42[E])),*E&=15))i(SP,(w(7),R&&--1[i]&&o?
R++,Q&&Q++,M--:0))DX(){$,O*=27840;O--;)O[(I*)k->pixels]=-!!(1<<7-O%8&r[O/2880*90+O%720/8+
(88+952[l]/128*4+O/720%4<<13)]);SDL_Flip(k);}main(BX,nE)n**nE;{9[i=E=r+P]=P>>4;$;q;)j[--q]=*++nE?
open(*nE,32898):0;read(2[a(I)*i=*j?lseek(*j,0,2)>>9:0,j],E+(M=256),P);$;Y=r+16*9[i]+M,Y-
r;Q|R||kb&46[E]&&KB)--64[T=1[O=32[L=(X=*Y&7)&1,o=X/2&1,l]=0,t=(c=y)&7,a=c/8&7,Y]>>6,g=~-T?y:
(n)y,d=BX=y,l],!T*t-6&&T-2?T-1?d=g:0:(d=y),Q&&Q--,R&&R--x(O=*Y,O=u=D(51),e=D(8),m=D(14)_
O=*Y/2&7,M+=(n)c*(L^(D(m)[E]|D(22)[E]|D(23)[E]^D(24)[E]))_ L=*Y&8,R(K(X)[r],=,c)_ L=e+=3,o=0,a=X
x a=m _ T(X[i])_ A(X[i])_ a<2?M(U,+=1-2*a+,P+24),v(f=1),G(S+1-a==1<<C-1),u=u&4?19:57:a-6?CX+2,a-
3||T(9[i]),a&2&&T(M),a&1&&M(P+18,=,U+2),R(M,=,U[r]),u=67:T(h[r])_(W=U B u=m,M-=~L,R(W[r],&,d)B 0
B L(=~)B L(=-),S=0,u=22,F(N>S)B L?c(I Z,i):c(I n,E)B/**/L?c(Z,i):c(n,E)B L?V(I Z,I,i):V(I n,I
Z,E)B L?V(Z,int,i):V(n,Z,E))_++e,h=P,d=c,T=3,a=m,M--_++e,13[W=h,i]=(o|=!L)?(n)d:d,U=P+26,M-
=~!o,u=17+(m=a)_(a=m B L(+=),F(N<S)B L(|=)B e(+)B e(-)B L(&=)B L(-=),F(N>S)B L(^=)B L(-),F(N>S)B
L(=))_!L?L=a+=8 x L(=):!o?Q=1,R(r[p=m x V],=,h):A(h[r])_ T=a=0,t=6,g=c x M(U,=,W)_(A=h(h[r]),V=m?
++M,(n)g:o?31&2[E]:1)&&(a<4?V%=a/2+C,R(A,=,h[r]):0,a&1?R(h[r],>>=,V):R(h[r],<<=,V),a>3?
u=19:0,a<5?0:F(S>>V-1&1)B R(h[r],+=,A>>C-V),G(h(N)^F(N&1))B A&=(1<<V)-1,R(h[r],+=,A<<C-
V),G(h(N*2)^F(h(N)))B R(h[r],+=(40[E]<<V-1)+,A>>1+C-V),G(h(N)^F(A&1<<C-V))B R(h[r],+=(40[E]<<C-
V)+,A<<1+C-V),F(A&1<<V-1),G(h(N)^h(N*2))B G(h(N)^F(h(S<<V-1)))B G(h(S))B 0 B
V<C||F(A),G(0),R(h[r],+=,A*=~((1<<C)-1>>V)))_(V=!!--1[a=X,i]B V&=!m[E]B V&=m[E]B 0 B
V=!++1[i]),M+=V*(n)c _ M+=3-o,L?0:o?9[M=0,i]=BX:T(M),M+=o*L?(n)c:c _ M(U,&,W)_
L=e+=8,W=P,U=K(X)_!R||1[i]?M(m<2?u(8,7,):P,=,m&1?P:u(Q?p:11,6,)),m&1||w(6),m&2||SP(1):0
_!R||1[i]?M(m?P:u(Q?p:11,6,),-,u(8,7,)),43[u=92,E]=!N,F(N>S),m||w(6),SP(!N==b):0 _
o=L,A(M),m&&A(9[i]),m&2?s(A(V)):o||(4[i]+=c)_ R(U[r],=,d)_ 986[l]^=9,R(*E,=,l[m?2[i]:(n)c])_
R(l[m?2[i]:(n)c],=,*E)_ R=2,b=L,Q&&Q++_ W-U?L(^=),M(U,^=,W),L(^=):0 _ T(m[i])_ A(m[i])_
Q=2,p=m,R&&R++_ L=0,O=*E,F(D(m+=3*42[E]+6*40[E])),z(D(1+m)),N=*E=D(m-1)_ N=BP(m-1)_ 1[E]=-h(*E)_
2[i]=-h(*i)_ 9[T(9[i]),T(M+5),i]=BX,M=c _ J(),T(V)_ s(A(V))_ J(),s((V&~m)+1[E])_ J(),l[E]=V _
L=o=1 x L(=),M(P+m,=,h+2)_++M,H(3)_ M+=2,H(c&m)_++M,m[E]&&H(4)_(c&=m)?
1[E]=*E/c,N=*E%=c:H(0)_*i=N=m&E[L=0]+c*1[E]_*E=-m[E]_*E=r[u(Q?p:m,3,*E+)]_ m[E]^=1 _ E[m/2]=m&1 _
R(*E,&,c)_(a=c B write(1,E,1)B time(j+3),memcpy(r+u(8,3,),localtime(j+3),m)),a<2?*E=~lseek(O=4[E]
[j],a(I)5[i]<<9,0)?((I(*)())(a?write:read))(O,r+u(8,3,),*i):0:0),O=u,D(16)?
v(0):D(17)&&G(F(0)),CX*D(20)+D(18)-D(19)*~!!L,D(15)?O=m=N,41[43[44[E]=h(N),E]=!N,E]=D(50):0,!++q?
kb=1,*l?SDL_PumpEvents(),k=k?k:SDL_SetVideoMode(720,348,32,0),DX():k?
SDL_Quit(),k=0:0:0;}i(G,48[E]=o)i(K,P+(L?2*o:2*o+o/4&7))
```

Software engineering

- Scientific and engineering software tools are first class research products!
- Programming is **not** software engineering

- This is what CHEME/CHEM/MSE 546 is about!

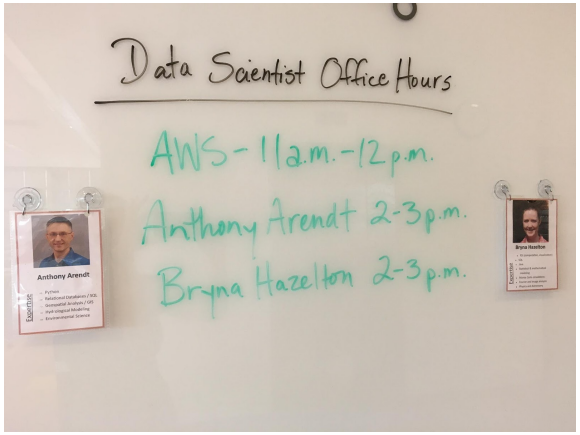
Data: Don’t be afraid of it!

DIRECT to the rescue!

- Data Science Option
  - Data Intensive Research Enabling Clean Tech (DIRECT)
    - ChemE 545
      - Data Science Methods for Clean Energy Research
    - ChemE 546
      - Software Engineering for Molecular Data Scientists
    - ChemE 547
      - Capstone Project in Molecular Data Science

eScience to the rescue!

- Data Scientist Office Hours
  - Get help with your data science questions
    - Data management
    - Machine learning
    - Statistics
    - Visualization
    - Software engineering



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Swipe right for Data Science[1]

Molecular Data Scientist
Knows thermodynamics **and** machine learning

1. Josh Smith

What is data science?

- Quick in class exercise
- Alone: Define Data Science by answering as many of the following questions as you can (write or type your answer)
  - What is Data Science?
  - What/who is a data scientist?
  - Why is Data Science a thing all of a sudden?
  - Why does Data Science matter, broadly, in my field of [*insert*]?
  - Why does Data Science matter, specifically, in my sub-discipline of [*insert*]?

- ~5 min working alone – take some notes!

What is data science?

- Quick in class exercise
- At your tables:
  - Introduce yourselves (1st names and departments)
  - Appoint 1 facilitator (soonest birthday, e.g. today) and 1 scribe (farthest birthday, e.g., yesterday)
  - Go around the table, each person answers each question, then move onto next question → OK if you didn't answer something
    - *What is Data Science?*
    - *What/who is a data scientist?*
    - *Why is Data Science a thing all of a sudden?*
    - *Why does Data Science matter, broadly, in my field of [insert]?*
    - *Why does Data Science matter, specifically, in my sub-discipline of [insert]?*
- ~10 min (I will flex time as needed)

Questions?

- Questions about DIRECT or DSMCER?

Acknowledgements

Beck Research Lab

- Pearl Philip (ChemE, GSK)
- Rahul Avadhoot (ChemE)
- Jiayuan Guo (ChemE)
- Alexey Gilman (ChemE, PhD)

Gut microbiome & health

- Jisun Paik (Comparative Medicine)

Showcase examples

- Elizabeth Nance (ChemE)
  - Chad Curtis (ChemE)
  - Mike McKenna (ChemE)
- Wes Tatum (MSE)
  - Luscombe (Chemistry)
- Jay Rutherford (ChemE)
  - Posner (ChemE + MechE)
- Blake Hough (ChemE, PhD)
  - Pfaendtner & Schwartz

NSF

Department of Energy, United States of America

Gordon and Betty Moore Foundation

Alfred P. Sloan Foundation

Fred Hutch University of Washington Cancer Consortium

eScience Institute
Advancing data-intensive discovery in all fields