Knowledge and solutions for a changing world

Be boundless

Advancing data-intensive discovery in all fields

# Data Science Methods for Clean Energy Research (DSMCER)

&

# Software Engineering for (SEMDS) Molecular Data Scientists

## UW DIRECT

(Data Intensive Research Enabling Cutting-edge Tech)

https://uwdirect.github.io


**Stéphanie Valleau**

Chemical Engineering

**Dave Beck (dacb)**

eScience/Chemical Engineering

# What is this class about?

Overview of **Data Science methods**

- Basics of statistics
- Tool selection
- Best practices
- Not about designing new algorithms

**Group project** using these methods

Provide you with computational tools and a computational mindset to tackle science problems

# Course website & setup

**Class website:** https://uwdirect.github.io

Let's go there now!

**Equipment / work platforms**

- Laptops: use them ☺!
- Slack: use it!
- Software: install it!

# Panopto recordings

- We will record all lectures using Panopto – these will include the speaker's screen and audio.

- For virtual lectures (first week), your names / chats and videos are not recorded – even when your videos are turned on!

# Code of Conduct

Please **read and make sure to respect the code of conduct**

https://uwdirect.github.io/code_of_conduct.html

If you find cases where the code of conduct is not being respected, let us know!

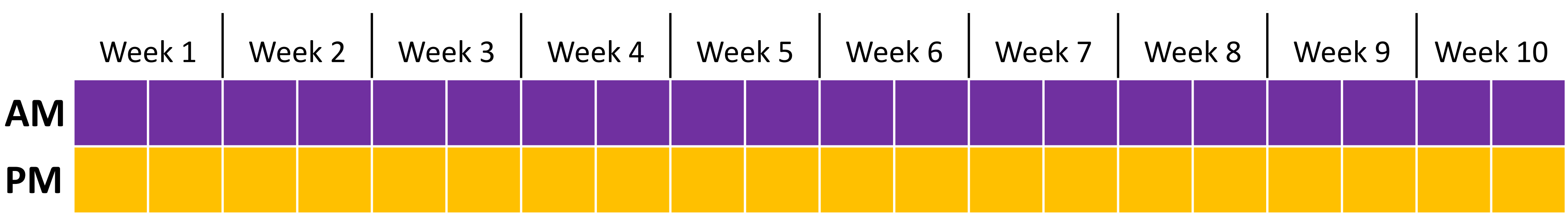
If you do not respect the code of conduct, we may refer to the university for action.

# Two quarters of courses in one!

- Two quarter courses make up training
  - CHEME 546: Software Engineering for Molecular Data Scientists (SEMDS)
    - One quarter (10 weeks)
  - CHEME 545: Data Science Methods for Chemical Engineering Research (DSMCER)
    - One quarter (10 weeks)
- UW runs these concurrently

SEMDS

DSMCER



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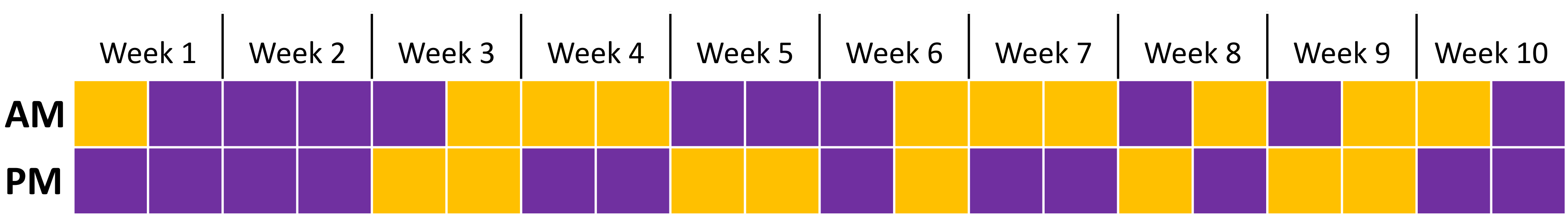
SEMDS

DSMCER



# About Stéphanie Valleau

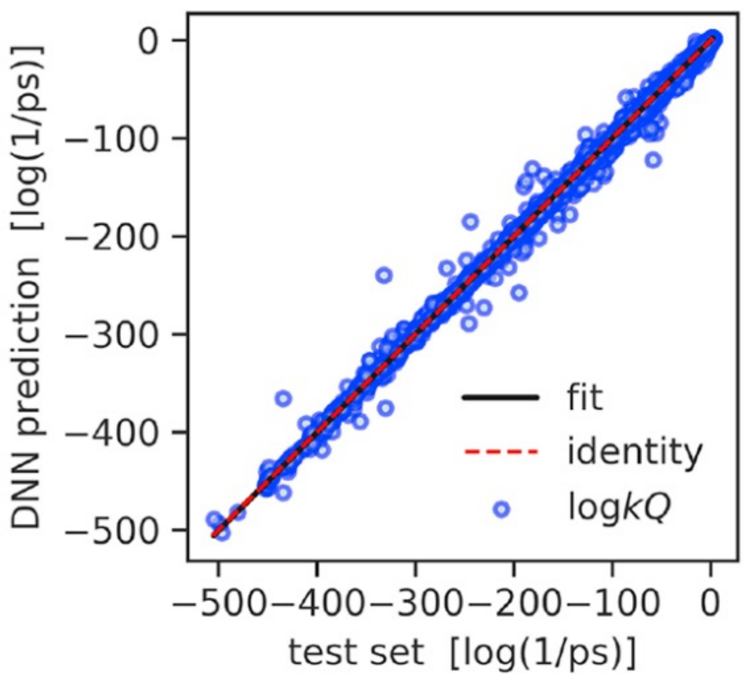

*Office*: Zoom and Slack
*Email*: valleau+dsms@uw.edu
*Group webpage:* valleau-lab.com

- **Background** – Chemistry (BS), Chemical Physics (MS, PhD), Physics (AM), Computer science (Secondary field)
- **Research** – Solve chemical problems using computers (no gloves ;) ) – kinetics / exciton transport – from ab initio to ML predictions

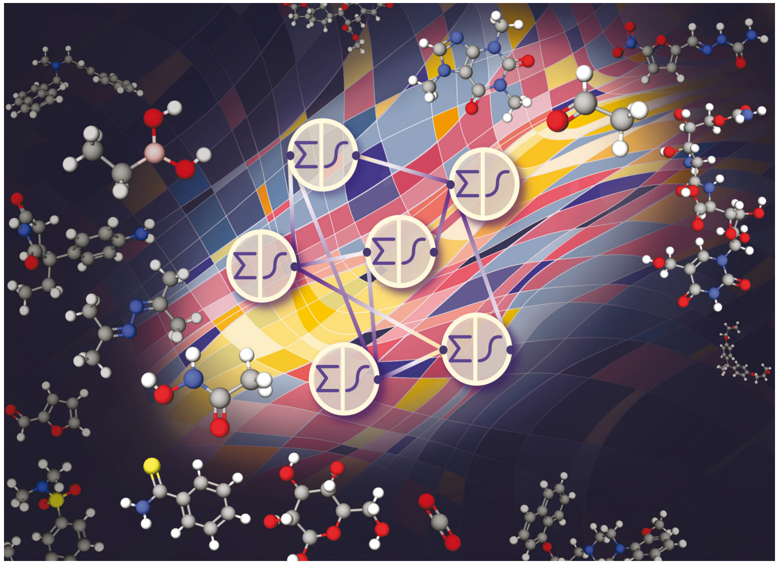
# Data science + Kinetics

Predict reactivity using machine learning, ML, algorithms – e.g. neural networks (large speedup – months to minutes)

Quantum rate constants [1]




Kinetics [2]



[1] Komp, E.; **Valleau, S.** *J. Phys. Chem. A.*, 124, 41, 8607–8613, 2020
[2] Komp. E; Janulaitis, N.; **Valleau, S.** *PCCP,* https://doi.org/10.1039/D1CP04422B, 2022

# About Dave Beck

- **Background** – Computer science, biology, chemistry (BS); Medicinal Chemistry (PhD); BioE (post-doc)
- **Research** – Molecular data science with applications in energy, environment and health. Scientific software engineering for reproducibility.
  - Molecular mechanics
  - *omics
  - ML in molecular settings

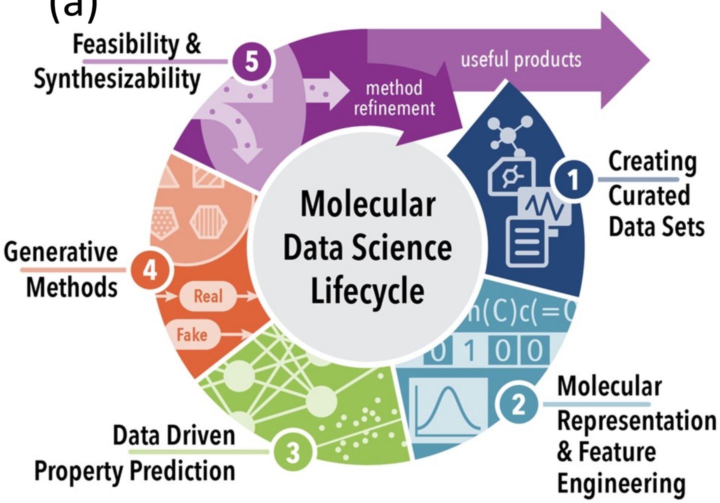
*Office*: Zoom and Slack

*Email*: [dacb@uw.edu](mailto:dacb@uw.edu)

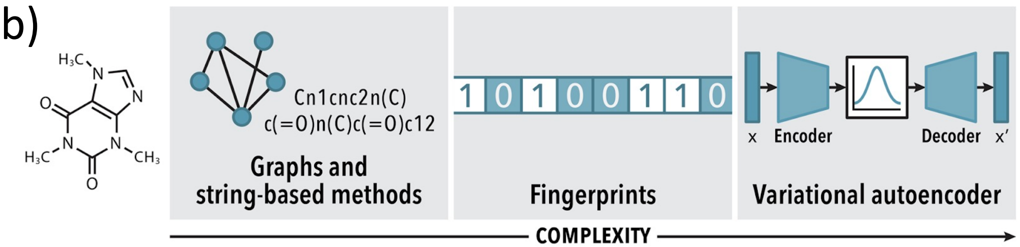
# Molecular Data Science

Combining (a) diverse data sources and unique (b) molecular representations and (c) generative models to design new molecules.

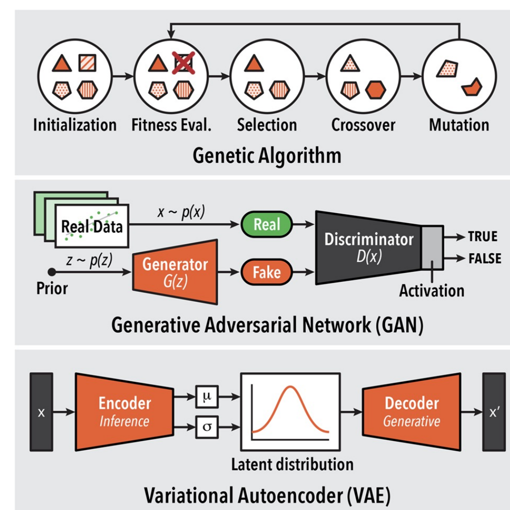
(a)




(b)




(c)




[1] Ashraf, Joshi, Beck, Pfaendtner. *Ann. Rev. Bio. Chem. Eng*. https://doi.org/10.1146/annurev-chembioeng-101220-102232

# About Evan Komp

*Office*: Zoom and Slack

*Email*: [evankomp@uw.edu](mailto:evankomp@uw.edu)

- I am concerned with leveraging machine learning to predict kinetic parameters allowing for speedy design of gas phase systems such as carbon capture in flue gas or precursor in chemical vapor manufacturing techniques. I am super excited to develop tools bringing the informatics of data science to kinetics design and to drive the community in terms of minimizing waste and energy use.

# About Nisarg Joshi

- I'm a third year PhD student in Pfaendtner Research Group. I use neural networks for my research to study simulations. Excited to be a part of DIRECT again! **Data Science rocks!!**

*Office*: Zoom and Slack
*Email*: nisargj@uw.edu

# Data + science?


## Science, Art & Engineering

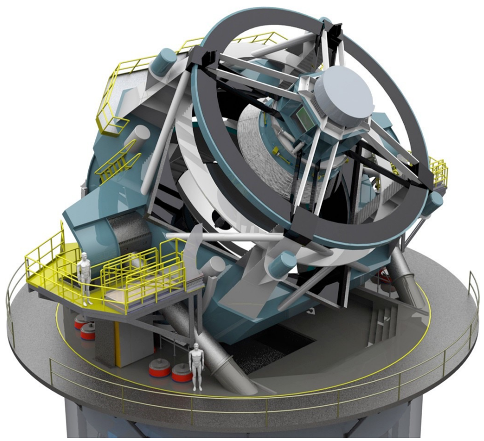
– **Physical Sciences**: Physics, Chemistry, Biology, Molecular science

– **Engineering**: Environment, Materials, Civil, Electrical

– **Social Sciences:** Psychology, Economics, Sociology, Public Policy

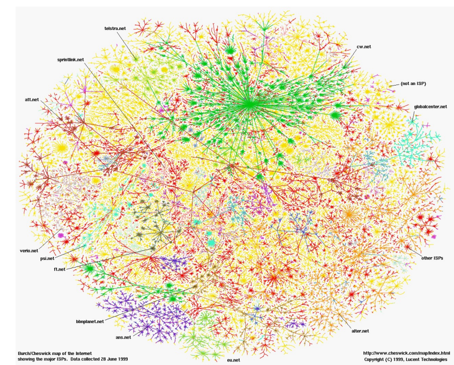
# OMG, so much data!

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



Astronomy: LSST

Physics: LHC



Sociology: Social networks

Biology: Sequencing

Neuroscience: EEG, fMRI

Economics: POS terminals

# Computers then and now

## 1943

**ENIAC** - Electronic Numerical Integrator and Computer

- High-speed memory - 20 words (equivalent to about **80 bytes**)
- simple calculations involving 20 numbers of ten decimal digits
- add and subtract **5000 times per second**

https://en.wikipedia.org/wiki/Computer#First_computing_device

## 2018


**SUMMIT - $2^{nd}$** fastest in the world

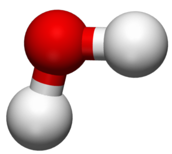
- Non-volatile memory per node **1600 gigabytes GB**
- mathematical calculations at the rate of **200 quadrillion per second**, or 200 petaflops

https://www.olcf.ornl.gov/summit/

# Where does all the data come from?

## Tracking the motion of molecules (data points)

chemistry / chemical engineering / material science



1 water molecule

- 3 atoms (*N*)
- $3N - 6 = 9 - 6 =$ **3** degrees of freedom to describe it

1 glass of water

- $N_{avogadro}$ molecules $\sim 6 \cdot 10^{23}$
- $(3N_{atoms} - 6)\, N_{avogadro} =$ $\mathbf{18 \cdot 10^{23}}$ degrees of freedom to describe it

```
array([[-7.23537334e-01,  5.75993650e+00, -4.16987014e-01],
       [ 2.39651691e+00,  3.26835346e+00,  5.03058537e-02],
       [ 3.72107558e+00,  8.35172720e+00,  2.69980407e+00],
       [ 1.98383469e+00, -5.97100116e-01, -3.30870629e+00],
       [ 8.62234431e+00,  4.20908286e+00,  4.17297967e+00],
       [ 3.18218791e+00, -1.69443169e+00,  6.29690948e-01],
       [ 5.14876585e+00,  3.74617250e+00,  5.53652032e+00],
       [ 3.38591148e+00,  2.14315223e+00, -2.58411138e+00],
       [illegible]
       [illegible]
       [ 2.16419342e+00, [illegible],  3.13175607e+00],
       [-3.26291521e+00, [illegible],  3.79147188e+00],
       [ 4.93178455e+00,  5.17781881e-01,  3.79143485e+00],
       [ 3.97577887e+00,  7.95303007e+00,  2.75966710e+00],
       [ 4.50534214e+00, -1.12475000e+00,  1.79212511e+00],
       [ 5.51834616e+00,  4.28598210e+00,  6.02622969e+00],
       [ 1.24097493e+00,  3.14230631e-01, -2.20149597e+00],
       [ 5.60820816e+00,  1.10054202e+00,  2.35192552e+00],
       [ 4.77062865e+00,  9.95839225e-01,  3.76613525e+00],
       [-1.58688321e+00,  5.02064104e+00,  5.90980561e+00],
       [ 1.44315688e+00, -6.24222044e-02, -1.81561712e+00],
       [ 2.49731088e+00,  3.96388958e+00, -1.45702882e+00],
```

**Many positions!!! (data!)**

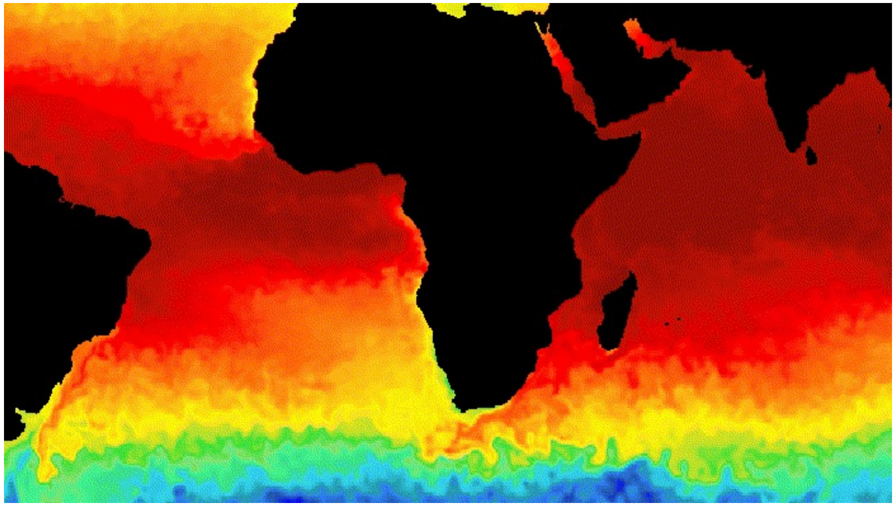
**X Y Z**

# Where does all the data come from?

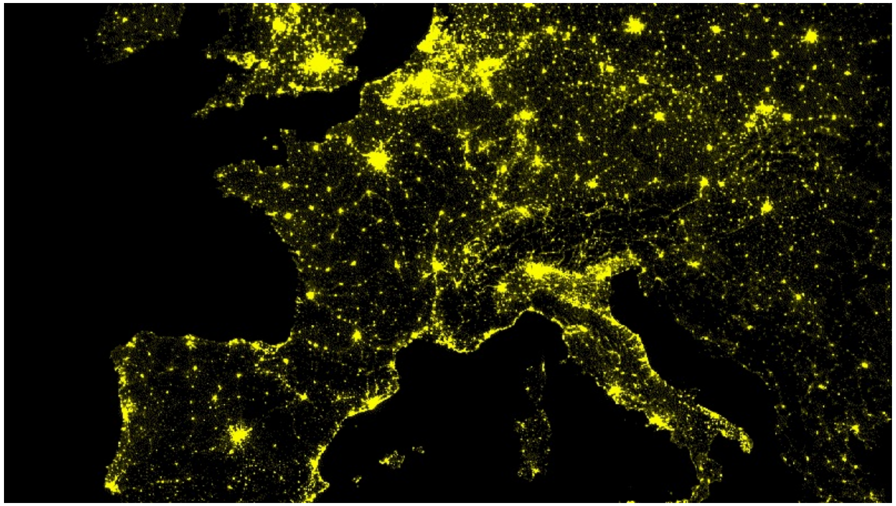
Satellite **images** / Measurements (**images**)

See e.g. 40 years of data made available here

https://developers.google.com/earth-engine/datasets



**Earth temperature**



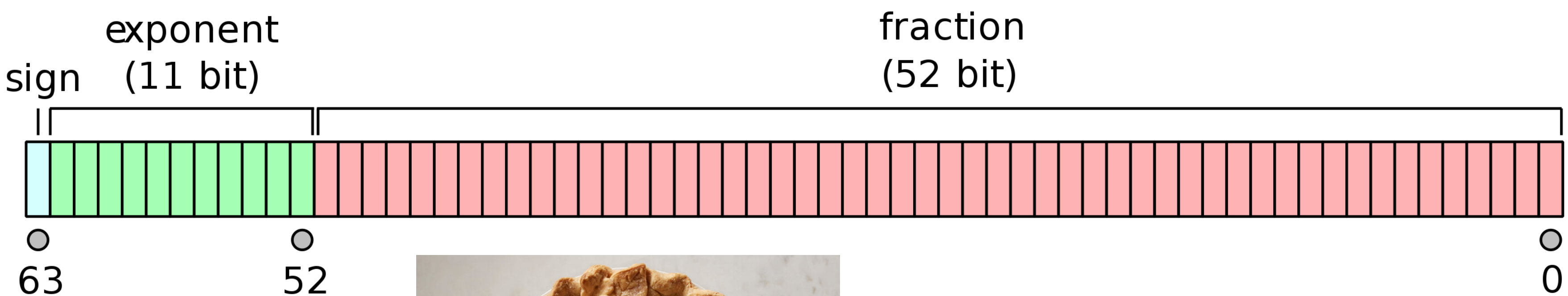
**Night time imagery**

Each image and data point occupies space “bytes” in a computer’s memory!

# Need memory to store data

One double precision number (16 significant figures) needs 64 bits – 8 bytes

3.141592653589793115997963468544185161590576171875



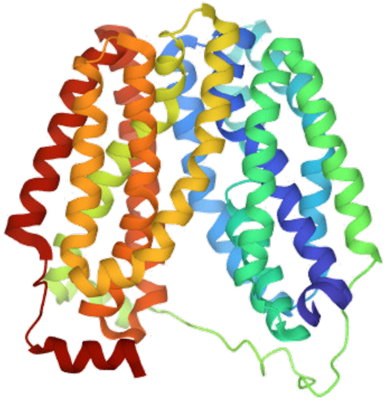

$\pi$

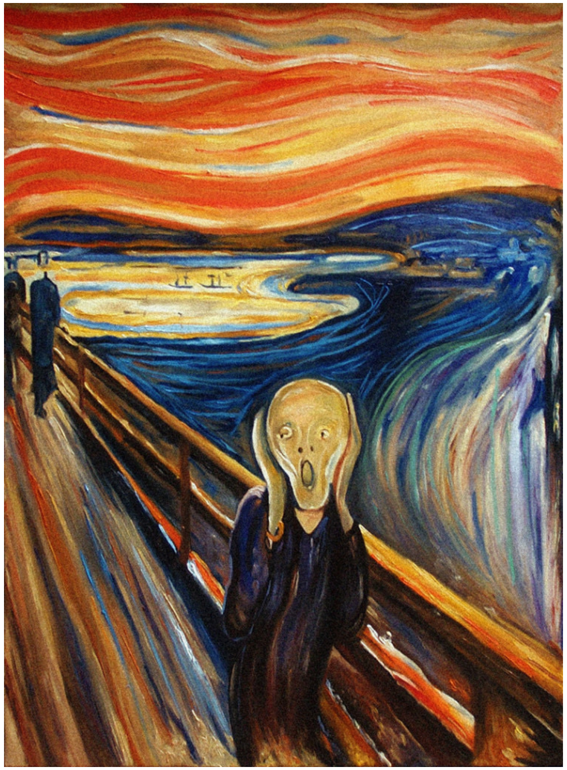
# Ok so for $N_{av}$ molecules????

We just need 18E+23 numbers to be stored so ….

## 1440000000000 Terabytes

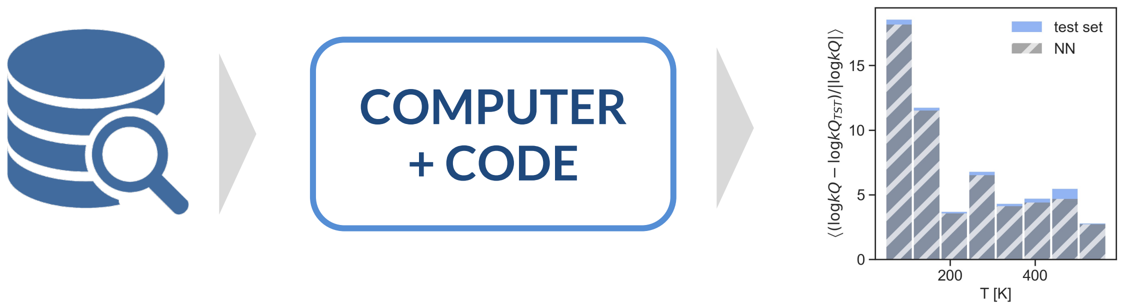
Even for a single protein we need to store a lot of data e.g. lactose permease 1PV6 – 6580 atoms – **138 kilobytes KB**





# Memory & time to compute

Now we want to **model** or **visualize** our data




- **Modeling data** – load data in e.g. lists, vectors, matrices and apply mathematical operations / functions on the data such as sums, products etc.

- **Visualizing data** – load data in e.g. lists, vectors, matrices and convert it into a graphical representation
- When we load data, it is stored in **random access memory RAM** – the larger the dataset the more memory we need.

# Memory & time to compute

**Modeling data – the larger the data the more time needed to carry out an operation**

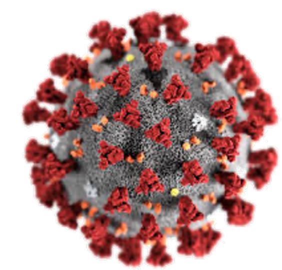
- Scalar multiplication - $1.0 \cdot 2.0$
- Vector multiplication – $[1.0\ 2.0\ 3.0 \ldots] \cdot [2.3\ 4.5\ 5.2 \ldots]$

**Time 1 ≪ Time 2**

- For vector of length $N$, when carrying out the dot product we make $N \cdot N$ multiplications and sum $N$ numbers afterwards

# Challenges

Evaluating models, extracting properties from/using large dataset is **computationally demanding: high memory cost** & **time demand**



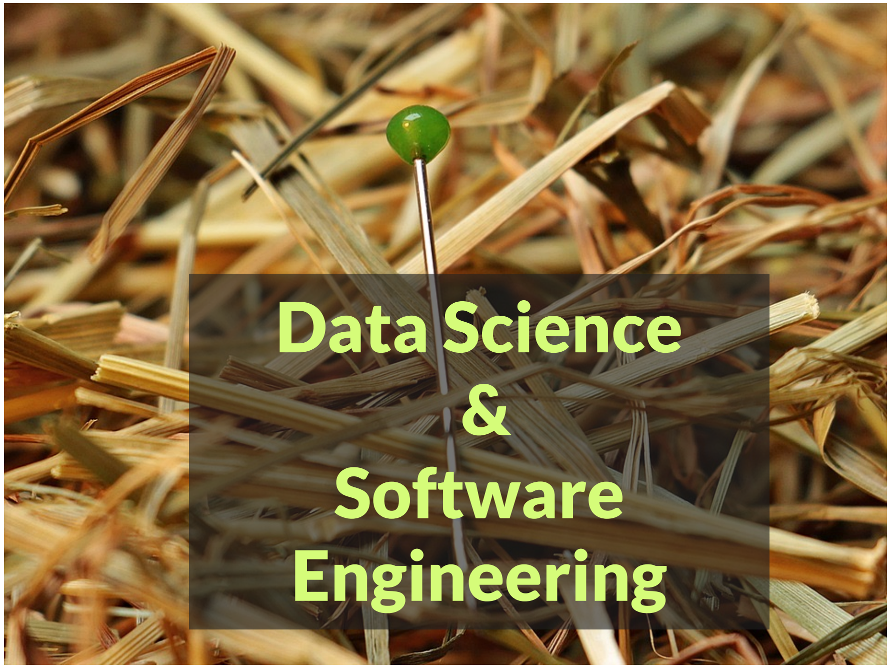
We need answers now for important problems

- Cure to COVID 19 / drug design
- Global warming - ecological forecasting
- Real-time sensing, learning, decision-making
- Detecting hazardous weather

Ref: The National Science Foundation's (NSF) Harnessing the Data Revolution (HDR) Big Idea

# Accelerating search & modeling?

How can we **rapidly and accurately** analyze large sets to extract / model what is of interest?



# 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

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)

Scalable data processing systems

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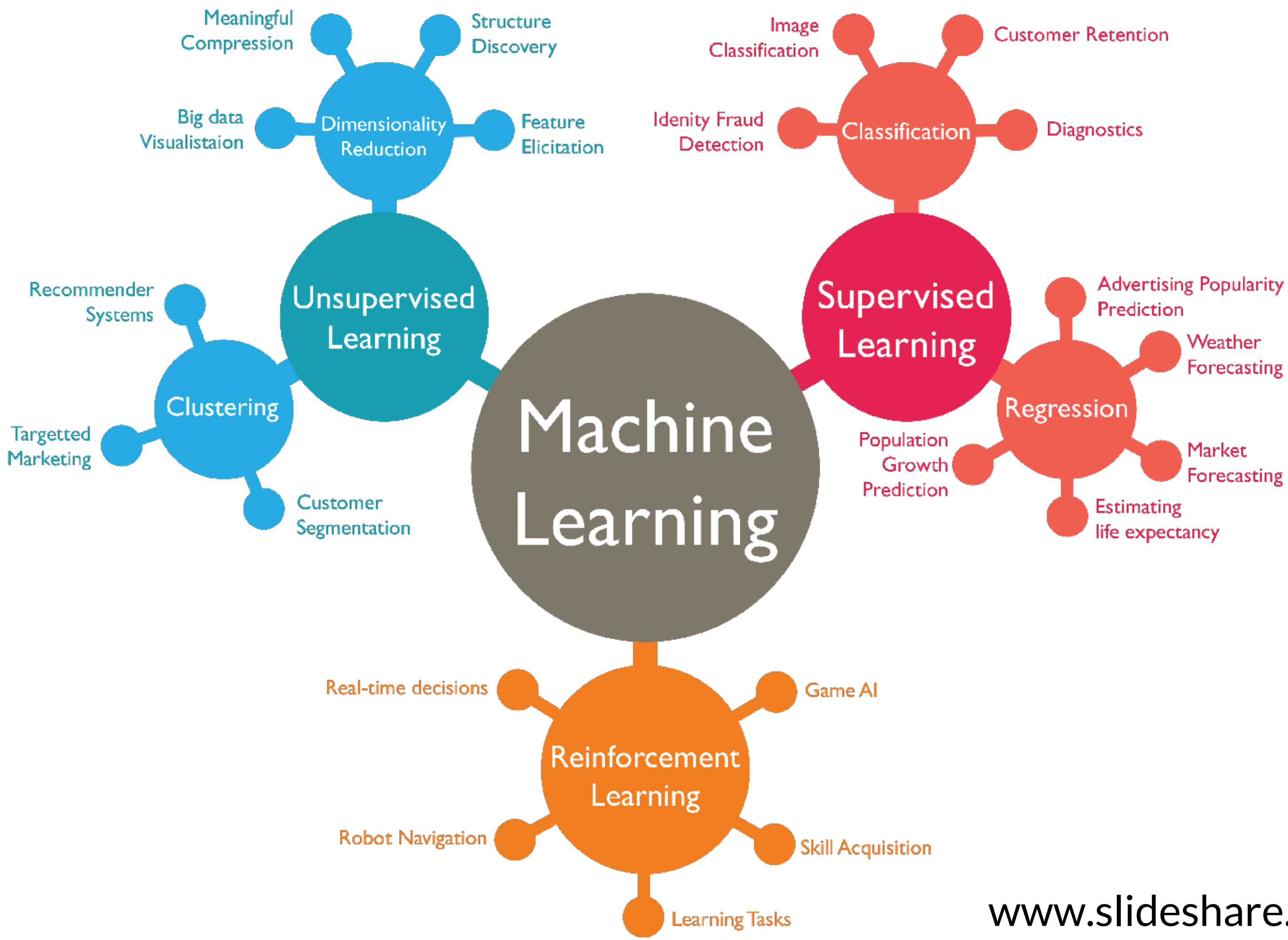
# Machine learning

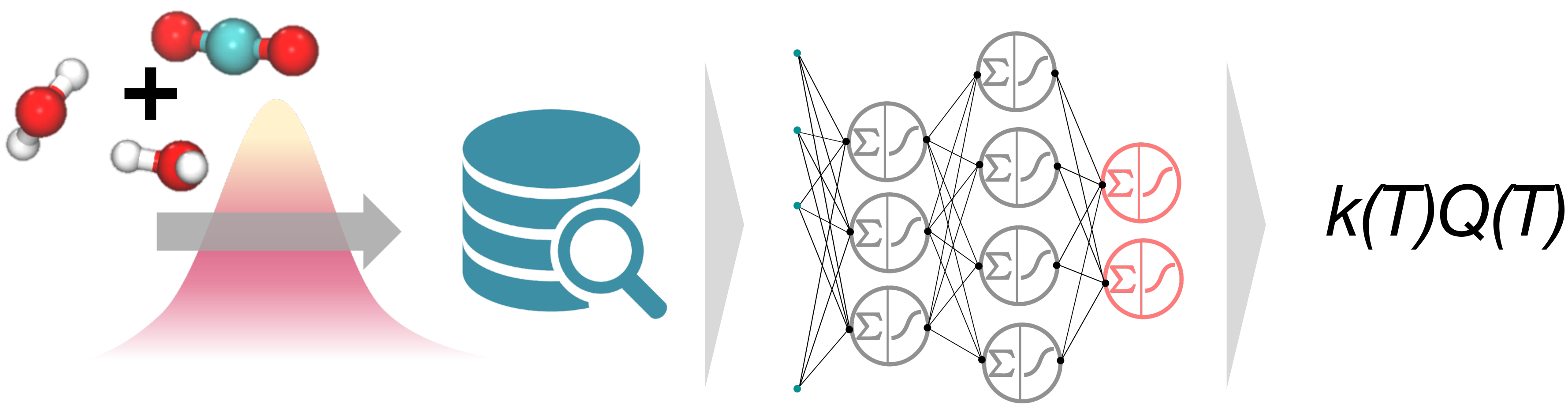



www.slideshare.net/awahid

# Machine learning

**Regression:** Predict a numerical response from input features

*Example*: predict reaction rate constant products k(T)Q(T) from a data set of 6.9 million data points





[1] Komp, E.; Valleau, S. *J. Phys. Chem. A.*, 124, 41, 8607–8613, 2020

# Machine learning

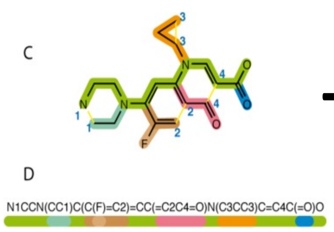
*Example*: predict binding affinity of small molecules to cancer drug target

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]

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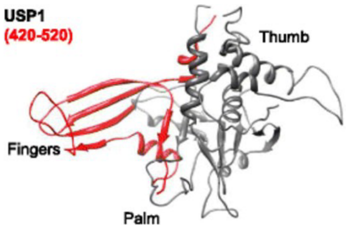


=?

Pearl Philip & Rahul Avadhoot

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

# Machine learning

*Example*: 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 |

# Machine learning

## Regression

Features or predictors

Outcome

| Molecule | Diffusion (nm/s) | Molecular Weight | C=C bonds | H-bond donors | H-bond acceptors | Kd (fM) |
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| 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 |
| New! | 6 | 121 | 1 | 0 | 0 | ??????? |

# 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)

| 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 |
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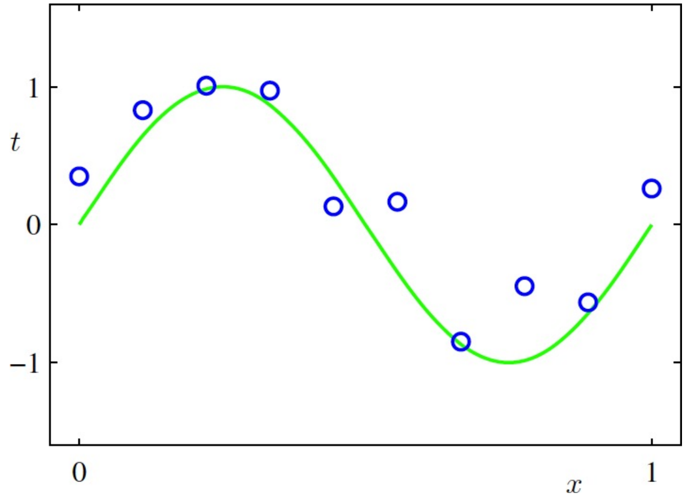
| 7 | 6 | 94 | 2 | 0 | 1 | 2 |
| 8 | 3 | 96 | 1 | 2 | 1 | 2 |
| 9 | 7 | 57 | 3 | 1 | 1 | 6 |

# Machine learning

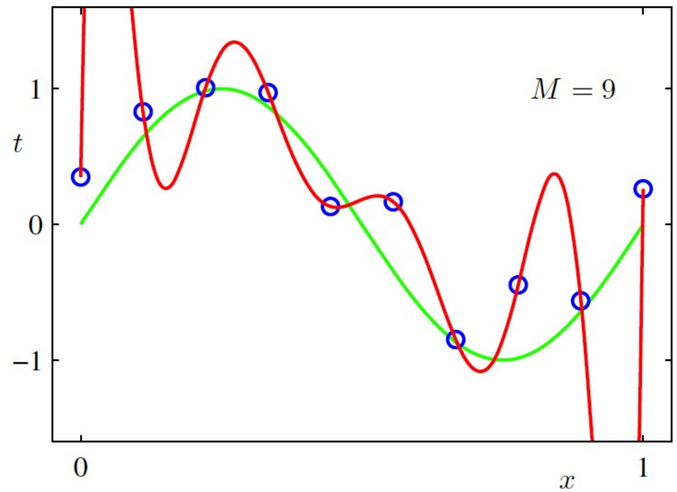
## Overfitting

"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(2πx)* + noise



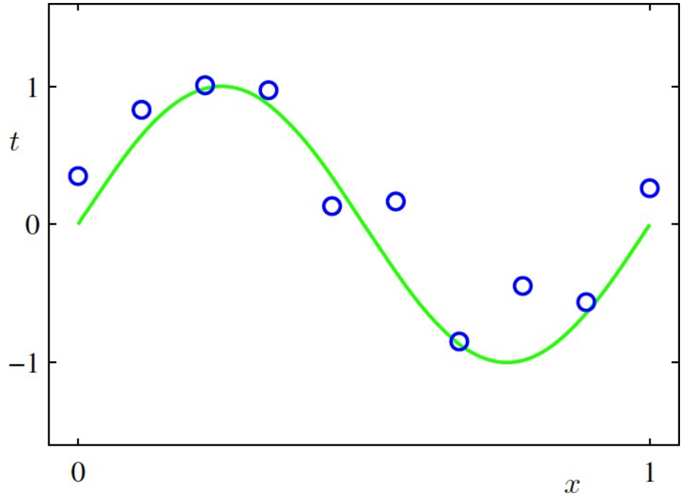

Fitting to points with a polynomial with order *M = 9*

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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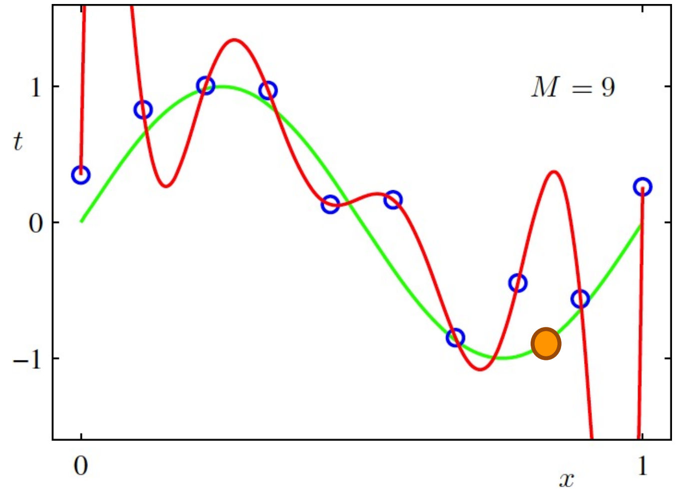


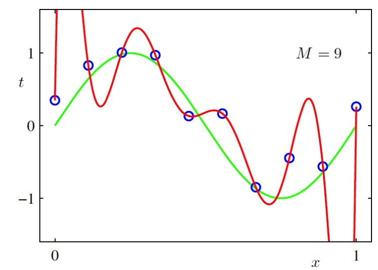

Fitting to points with a polynomial with order *M = 9*

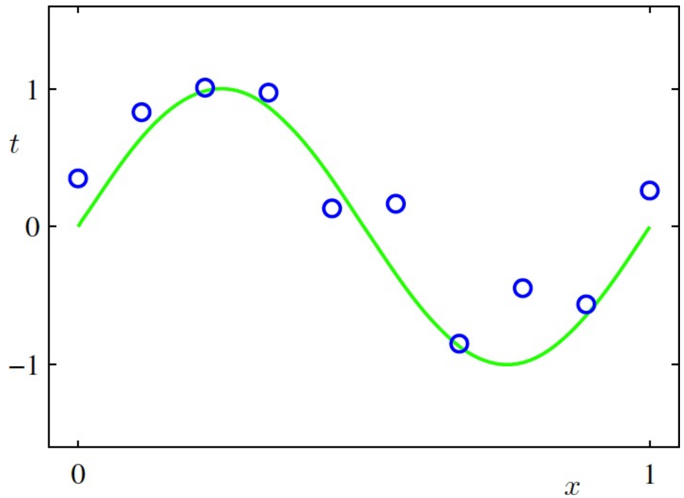
Pattern Recognition and Machine Learning. Bishop, 2006.

# Machine learning

**Proper fitting**

- Still fits the training data
- Performs better on **new** data

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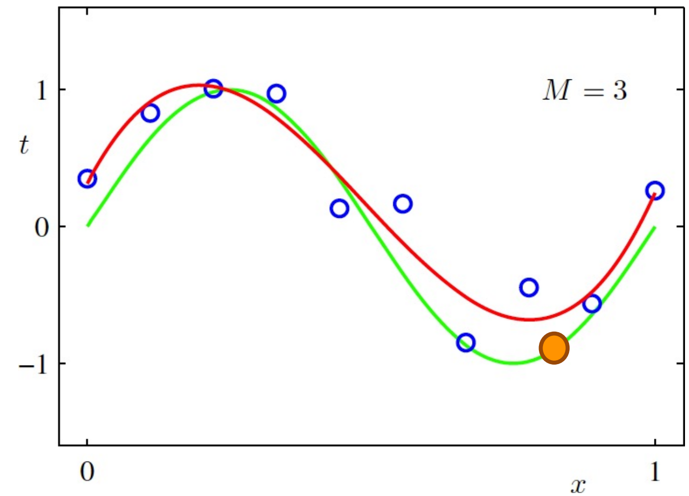


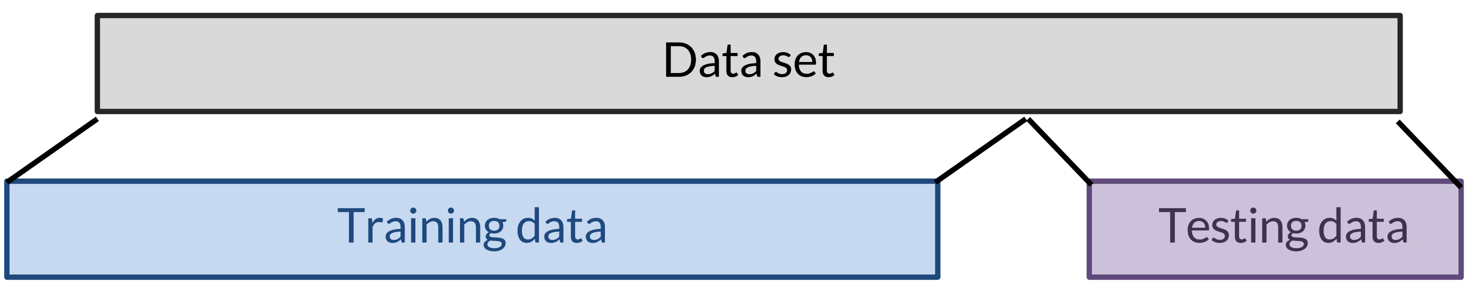

Fitting to points with a polynomial with order *M = 3*

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

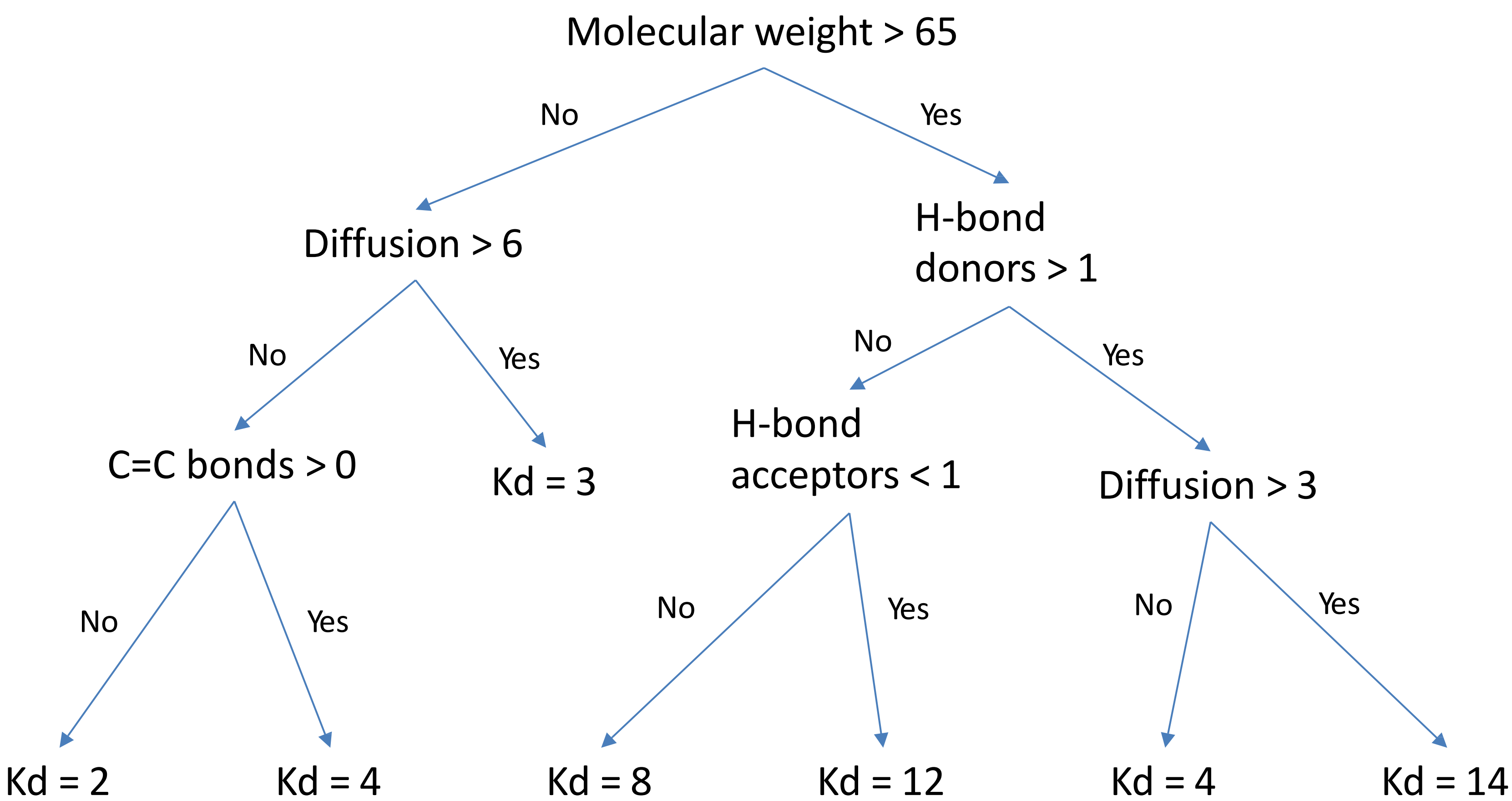



**Never ever ever ever ever** contaminate your model training with data from the test set!!!

# Machine learning

**Regression**

- Decision trees



# New paradigm of data-intensive discovery and innovation

**Deep domain knowledge**

**Data Science**

Data management

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Machine learning

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Statistics

Visualization

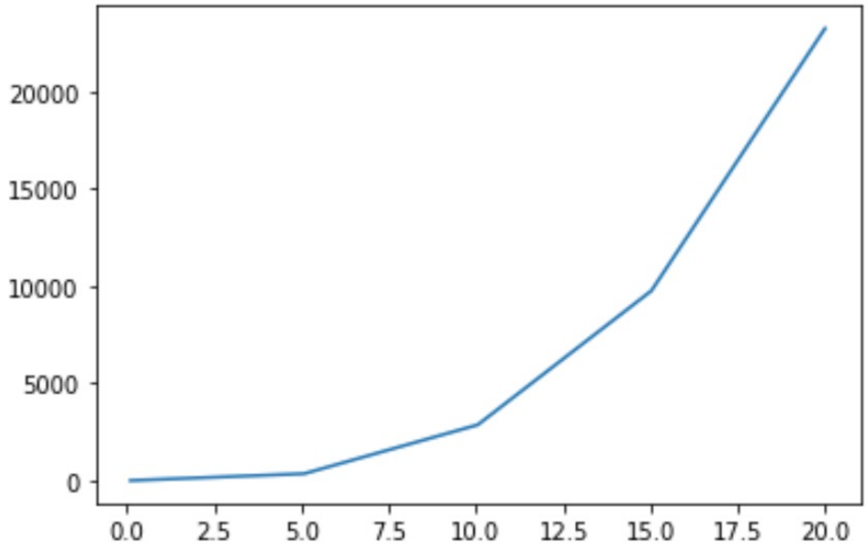
Software engineering

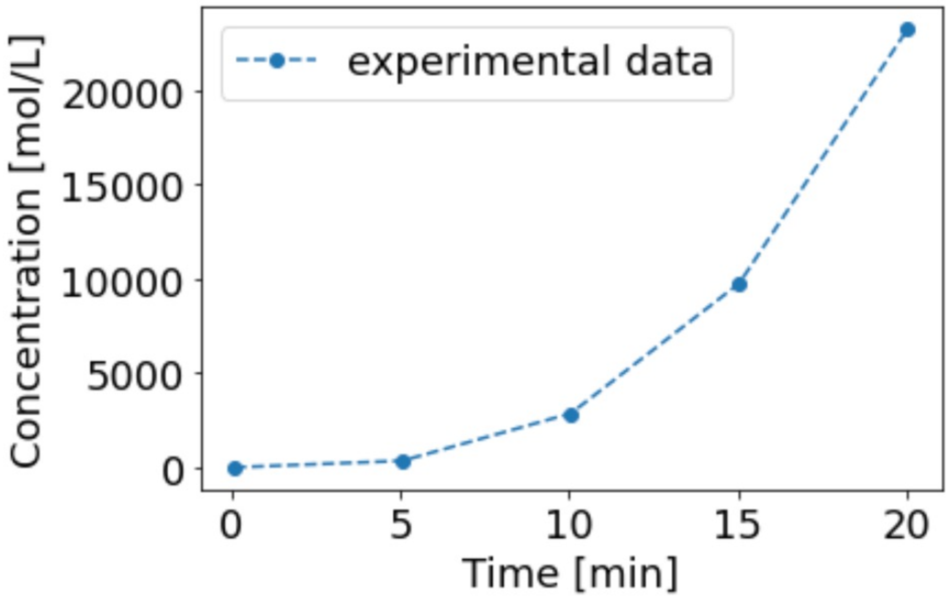
Molecular Data Scientist

Knows thermodynamics **and** machine learning

# Visualization

How can we clearly and accurately represent data?



# 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

# 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(),1[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!

# Meet each other!

**The best way to learn is from each other!**

We will now move you to a breakout room ☺

- 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 of the following questions, then move onto next question.
    1. *What is Data Science?*
    2. *What/who is a data scientist?*
    3. *Why is Data Science a thing all of a sudden?*
    4. *Why does Data Science matter, broadly, in my field of [insert]?*
    5. *Why does Data Science matter, specifically, in my sub-discipline of [insert]?*

# What did you think?

Facilitator & scribe give us your update!

# Data: Don't be afraid of it!

# DIRECT to the rescue!

**Data Science Option**

Data Intensive Research Enabling Clean Tech (DIRECT)

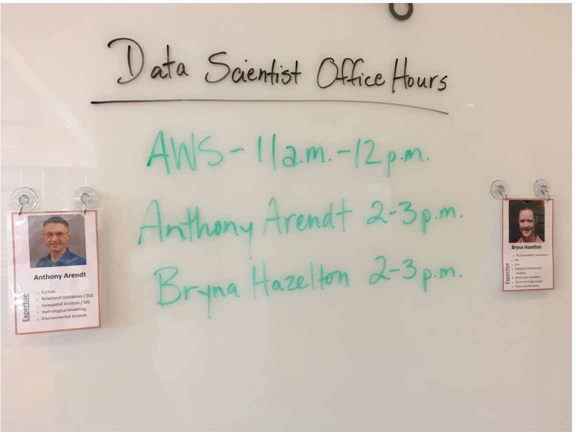
- ChemE 545: Data Science Methods for Clean Energy Research
- ChemE 546: Software Engineering for Molecular Data Scientists
- ChemE 547: Capstone Project in Molecular Data Science

# 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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# 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!

# Zoom chat your responses

After 5min we will ask you to write some responses to each question and share them with others

# Questions?