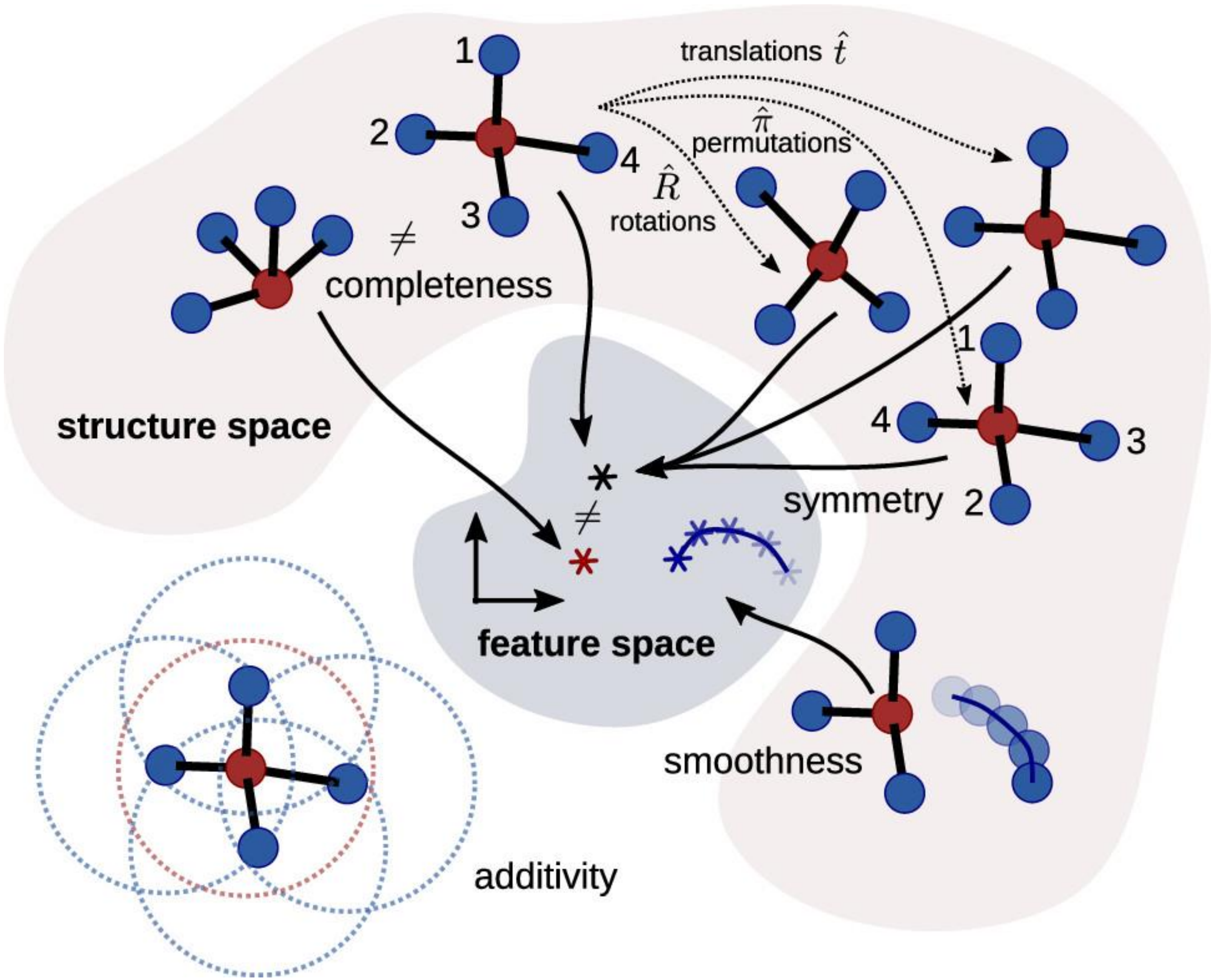
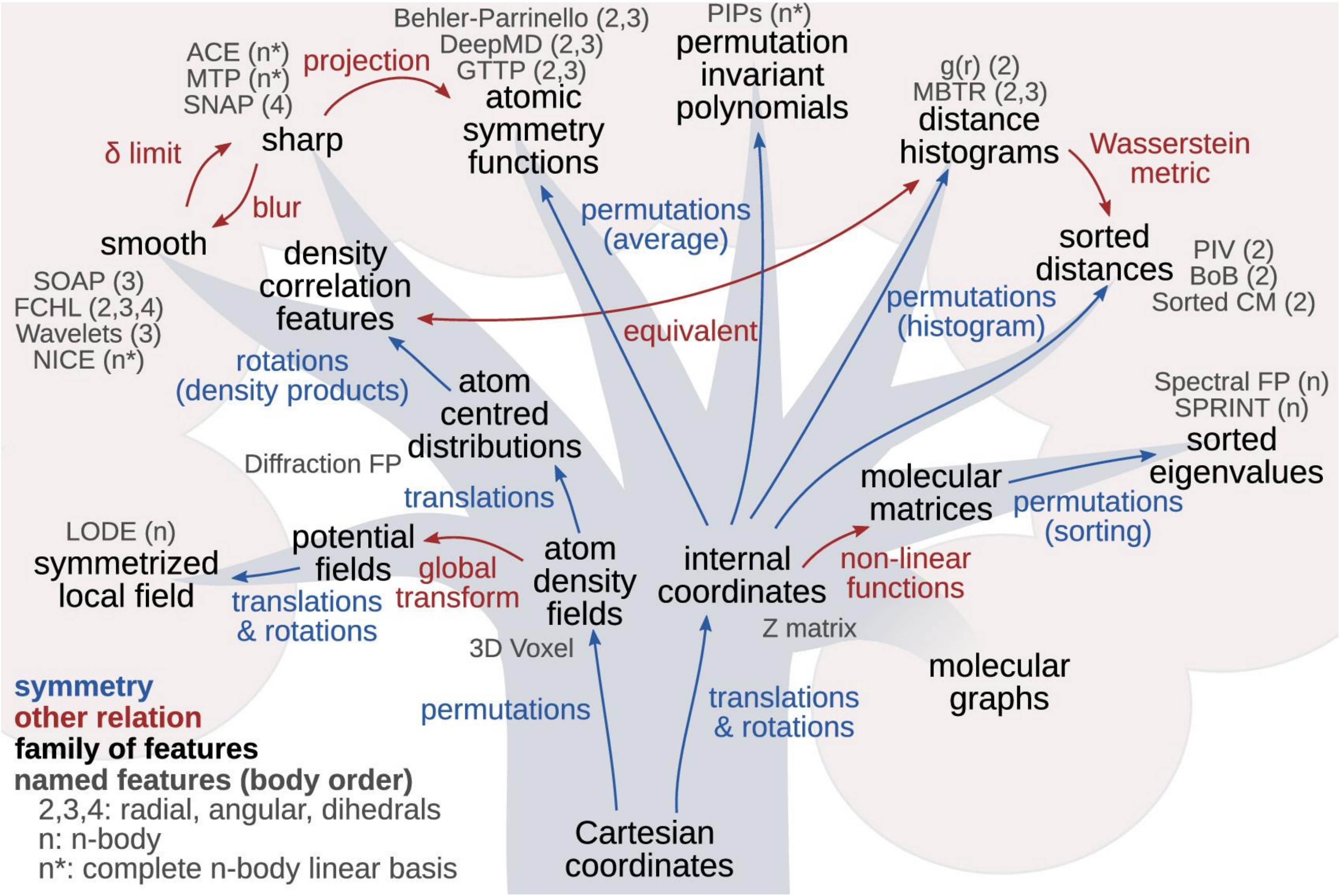
Representations

Requirements



Musil et al., *Chem Rev*, 2021.

Overview



ACE (n*)
MTP (n*)
SNAP (4)
sharp

projection

Behler-Parrinello (2,3)
DeepMD (2,3)
GTTP (2,3)
atomic symmetry functions

PIPs (n*)
permutation invariant polynomials

g(r) (2)
MBTR (2,3)
distance histograms

Wasserstein metric

δ limit

blur

smooth

SOAP (3)
FCHL (2,3,4)
Wavelets (3)
NICE (n*)

density correlation features

permutations (average)

equivalent

permutations (histogram)

sorted distances

PIV (2)
BoB (2)
Sorted CM (2)

rotations (density products)

atom centred distributions

Spectral FP (n)
SPRINT (n)
sorted eigenvalues

Diffraction FP

translations

molecular matrices

permutations (sorting)

LODE (n)
symmetrized local field

potential fields

global transform

translations & rotations

atom density fields

internal coordinates

non-linear functions

Z matrix

3D Voxel

molecular graphs

permutations

translations & rotations

Cartesian coordinates

symmetry
other relation
family of features
named features (body order)
2,3,4: radial, angular, dihedrals
n: n-body
n*: complete n-body linear basis

Musil et al., *Chem Rev*, 2021.

Compact Representations Useful

Expected error given sufficient data

$$\exp(-c/h_{X,\Omega})$$

Positive constant c

Function of the „fill distance“

$$h_{X,\Omega} \equiv \sup_{y\in\Omega} \min_{x_j\in X} \|y - x_j\|_2$$

Training data	X
Domain	Ω

Shorter fill distance: steeper learning curve, i.e. more data efficient model

Madych, Nelson, *J Approx Theory*, 1992.

Categorial: One-Hot

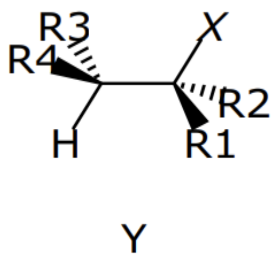
Categorial data vs regression

Solution: „binary“, „dummy“, „one-hot“ encoding

Encode *n* categories as vector of length *n-1* with one category (arbitrary) being the null vector.

Example:
- A: (0, 0)
- B: (1, 0)
- C: (0, 1)

Chemistry example: (ABBA|CD) -> (0,0,0,0,1,0,0,0,1,0,0,0,0,0,0,0|0,1,0,0,1)

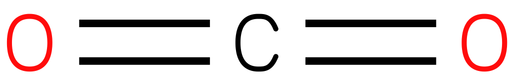


	A	B	C	D	E
R*k*	H	NO_2	CN	CH_3	NH_2
X	F	Cl	Br		
Y	H	F	Cl	Br	

GFvR, SN Heinen, M Bragato, Anatole von Lilienfeld, *Mach. Learn.: Sci. Technol.* 2020.

Graph-based

Often: molecules = well-defined bonds



Adjacency matrix

- 1 if atoms i and j are bonded
- 0 otherwise

$$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$$

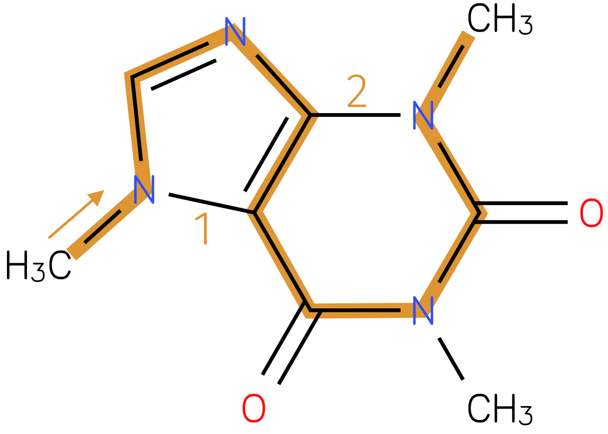
Bond order matrix

- Bond order if atoms i and j are bonded
- 0 otherwise

$$\begin{matrix} 0 & 2 & 0 \\ 2 & 0 & 2 \\ 0 & 2 & 0 \end{matrix}$$

SMILES

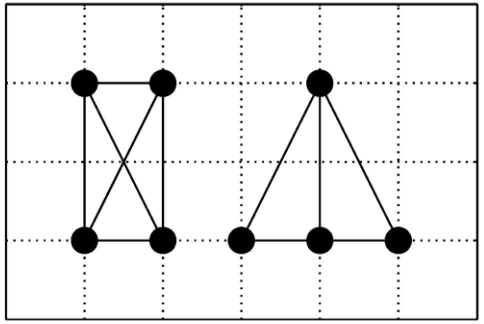
- Bonds: Nothing (1), = (2), # (3), $ (4)	O=C=O
- Partial charges	[Na+]
- Fragments: .	[Na+].[Cl-]
- Rings: labels	C1CCCCC1
- Branches: parentheses	



CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Distance-based

Many-body descriptions, e.g. all pairwise distances



	s	l	m
s		m	l
l	m		s
m	l	s	

	l	l	m
l		m	s
l	m		s
m	s	s	

Even three- and four-body interactions not unique [1].

Chemistry: **Coulomb Matrix [2]**

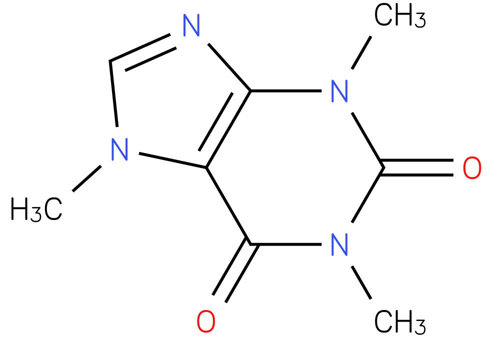
- Diagonal: $0.5Z_i^{2.4}$
- Off-diagonal: $Z_iZ_j/\|\mathbf{R}_i-\mathbf{R}_j\|$
- Problem: sorting, uniqueness

[1] Pozdnyakov et al., *Phys Rev Lett* 2020. [2] M. Rupp et al., *Phys Rev Lett* 2012.

Fingerprints

Collect relevant features of a molecule into a vector.

- Fixed list of functional groups (e.g. Joback method)
- Hash of generated circular atom environments (e.g. ECFP)
- Kinds of generated local environments (e.g. Morgan)
  - Element, # heavy neighbors, # protons, charge, part of ring...
- Fixed checklist of features (e.g. MACCS keys)
  - Subgraphs



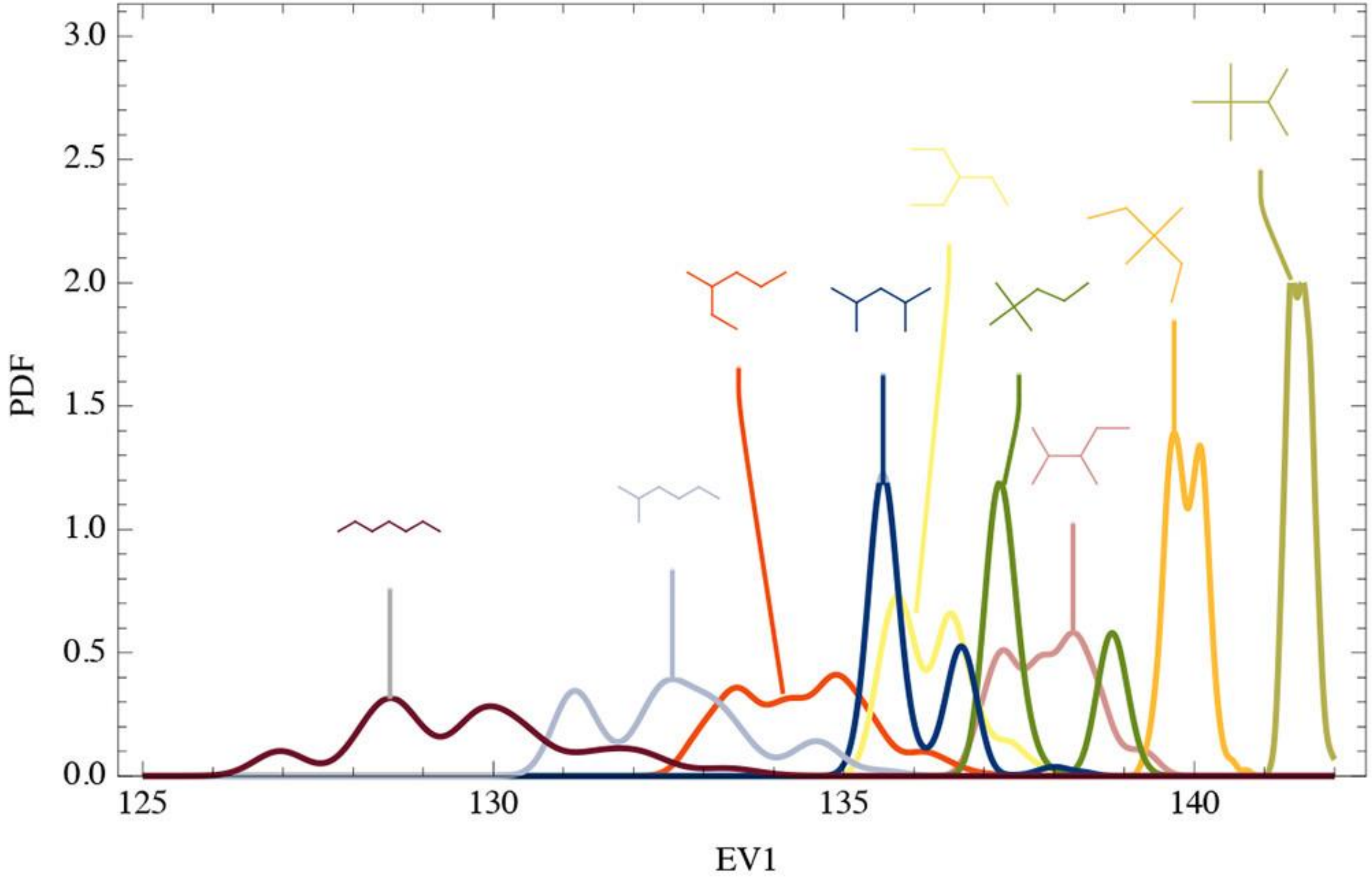
Morgan (feature: count)
10565946: 2, 348155210: 1, 476388586: 1, 540046244: 1, 553412256: 1, 864942730: 2, 909857231: 1, 1100037548: 1, 1333761024: 1, 1512818157: 1, 1981181107: 1, 2030573601: 1, 2041434490: 1, 2092489639: 3, 2246728737: 3, 2370996728: 1, 2877515035: 1, 2971716993: 1, 2975126068: 2, 3140581776: 1, 3217380708: 4, 3218693969: 1, 3462333187: 1, 3657471097: 3, 3796970912: 1

MACCS keys:
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 0,
0, 0, 1, 0, 0, 1, 1, 0, 1, 1, 1, 1, 0, 0, 1, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 1, 0, 0, 1, 1, 1, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0,
0, 0, 0, 1, 1, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 0]

Spectra

Condense a matrix into its eigenvalues

- No sorting issue, as permutationally invariant
- Smaller: N instead of N^2
- Lossy



J. Schrier, *J Chem Inf Model*, 2020.