Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression

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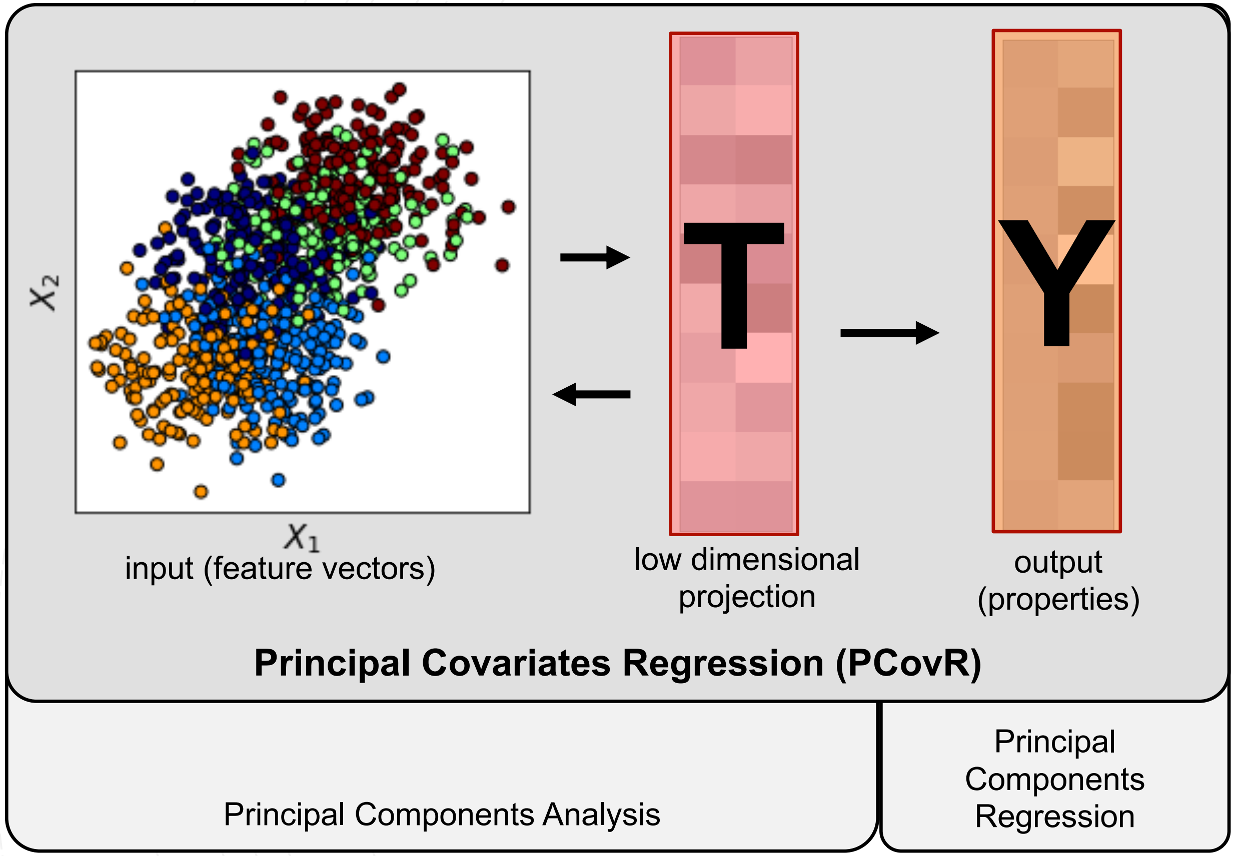
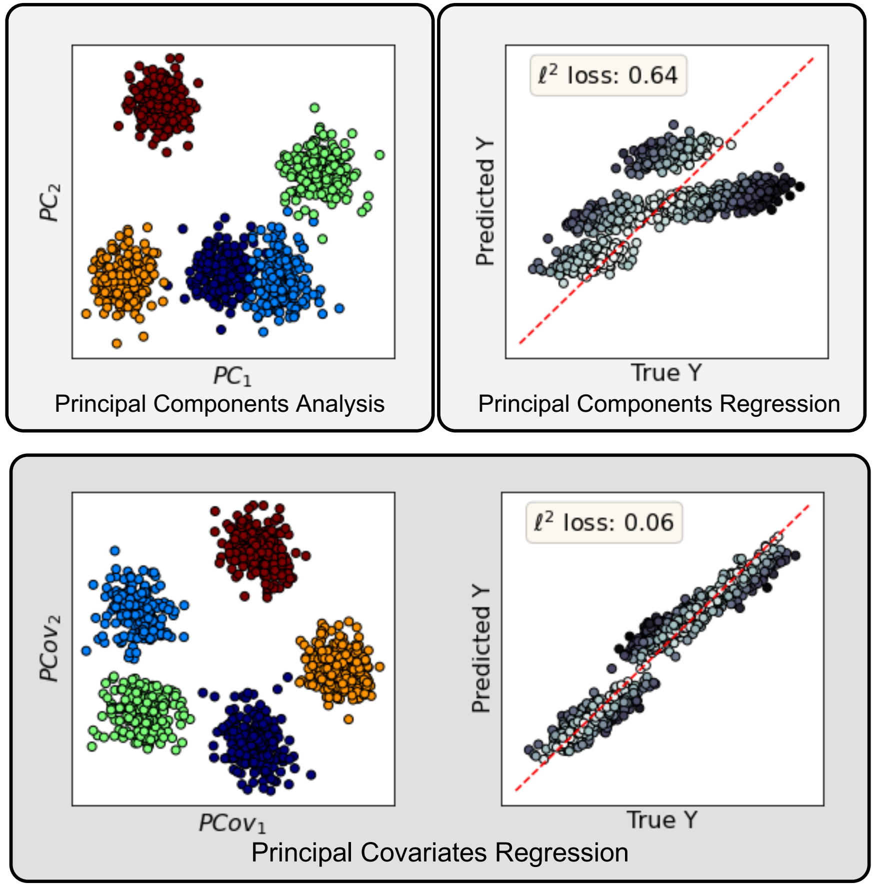
Principal Covariates Regression (PCovR)

is a dimensionality reduction technique that determines a latent-space projection that incorporate saspects of supervised learning.





S. de Jong, H.A.L. Kiers, Chemom. intell. lab. syst. 14 (1992) 155-164.
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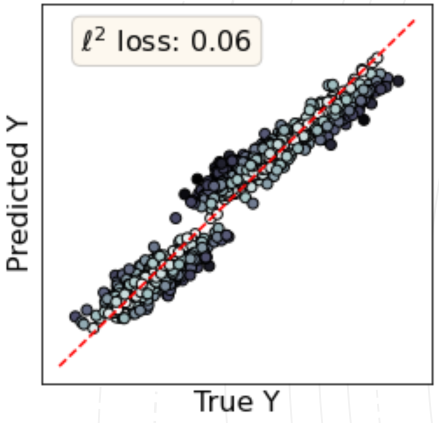
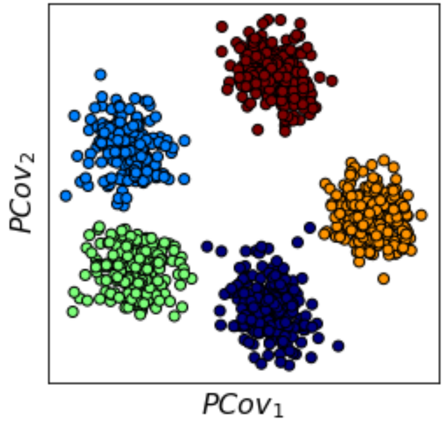
Inputs: sklearn.datasets.make_blobs
Regression Model: RidgeCV(cv=5)

Principal Covariates Regression (PCovR)

is controlled by a mixing parameter α that weights the regression and decomposition tasks.





$$\alpha = 0.5$$

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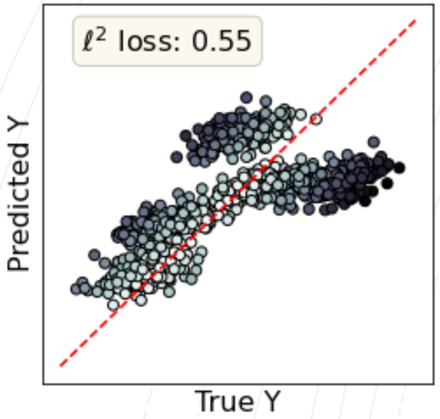

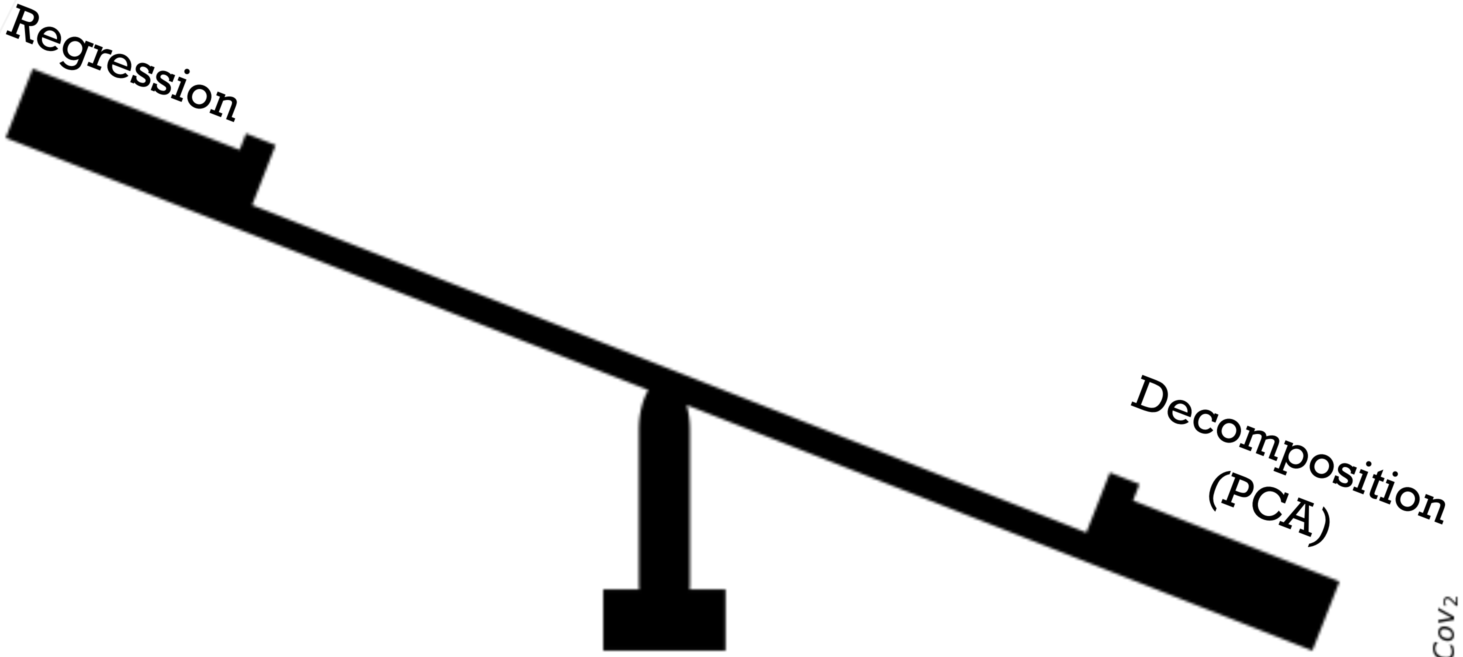

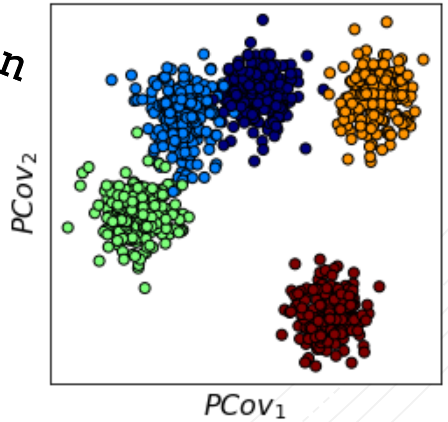

$\alpha = 0.9$

Principal Covariates Regression (PCovR)

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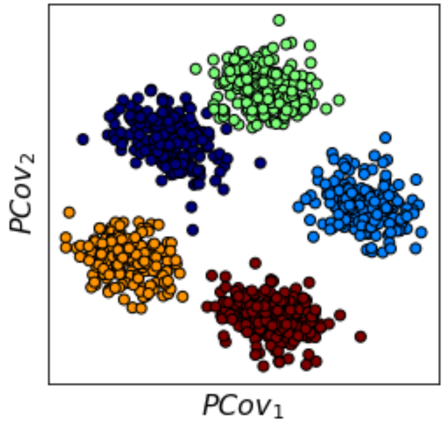
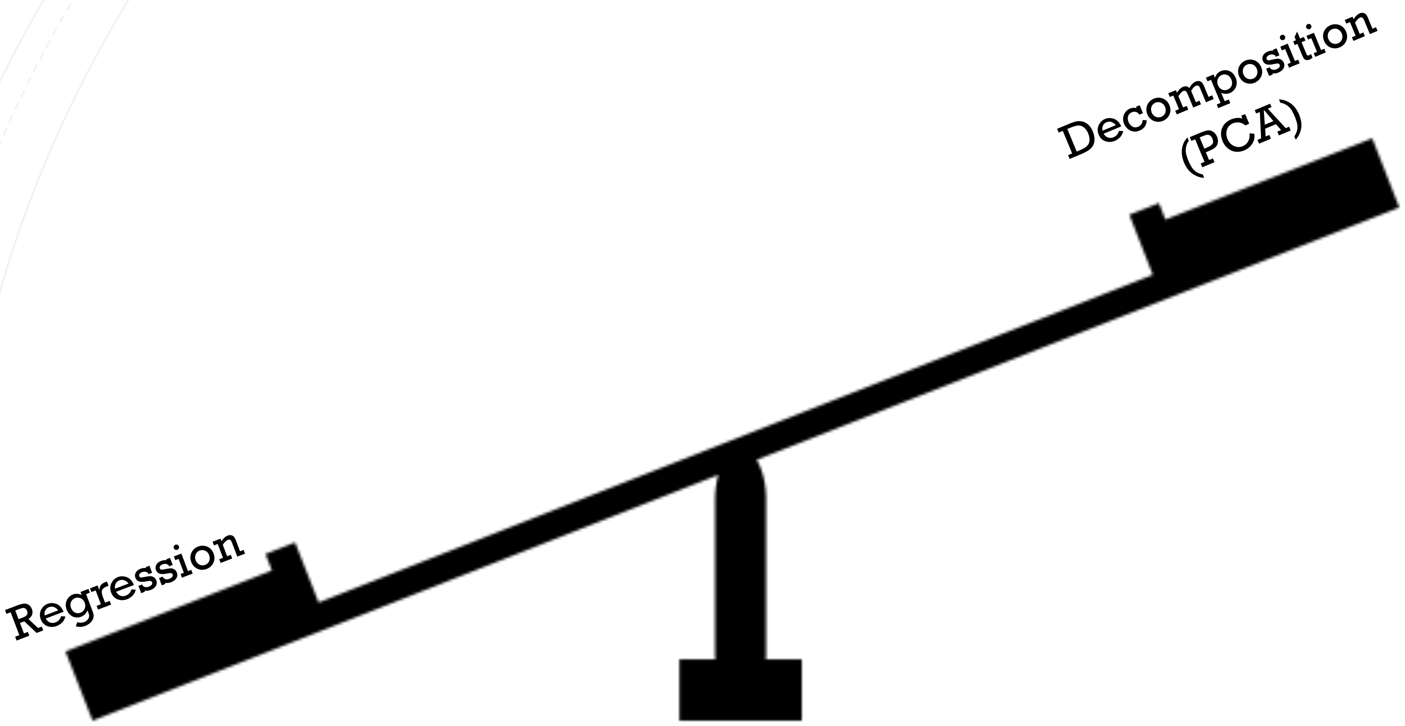
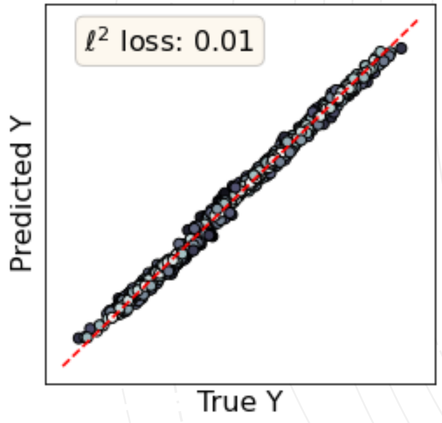


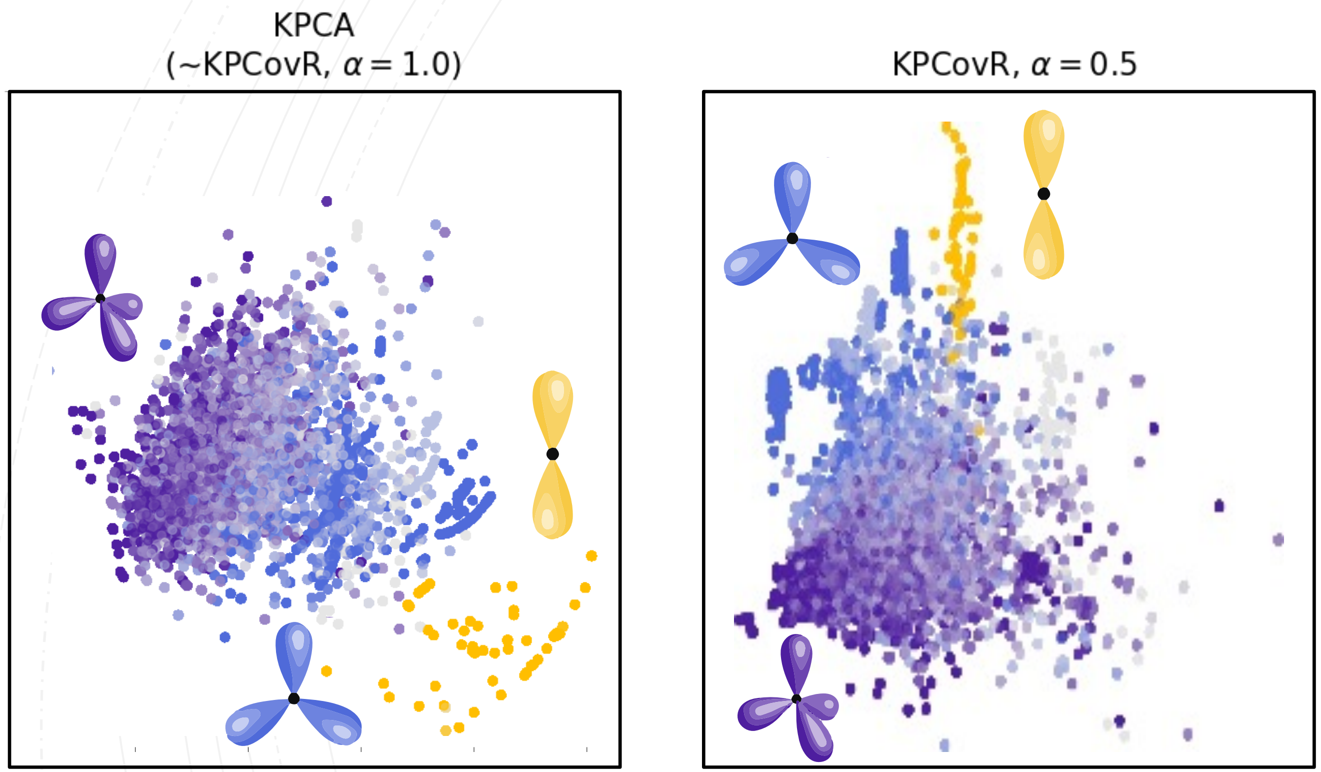




$\alpha = 0.1$

Kernel Principal Covariates Regression

Determines a low-dimension projection from a similarity kernel, considering target data when constructing the projection.



Inputs: SOAP features of 10,000 AIRSS carbon crystals
Target: energies in [eV / atom]
Kernel Parameters: RBF kernel, γ=$10^{-3.8}$
(1/1) train / test split

B. A. Helfrecht, **RKC**, G. Fraux, and M. Ceriotti. 2020 Mach. Learn.: Sci. Technol. 1 045021
C. J. Pickard. AIRSS Data for Carbon at 10GPa and the C+N+H+O System at 1GPa (2020).
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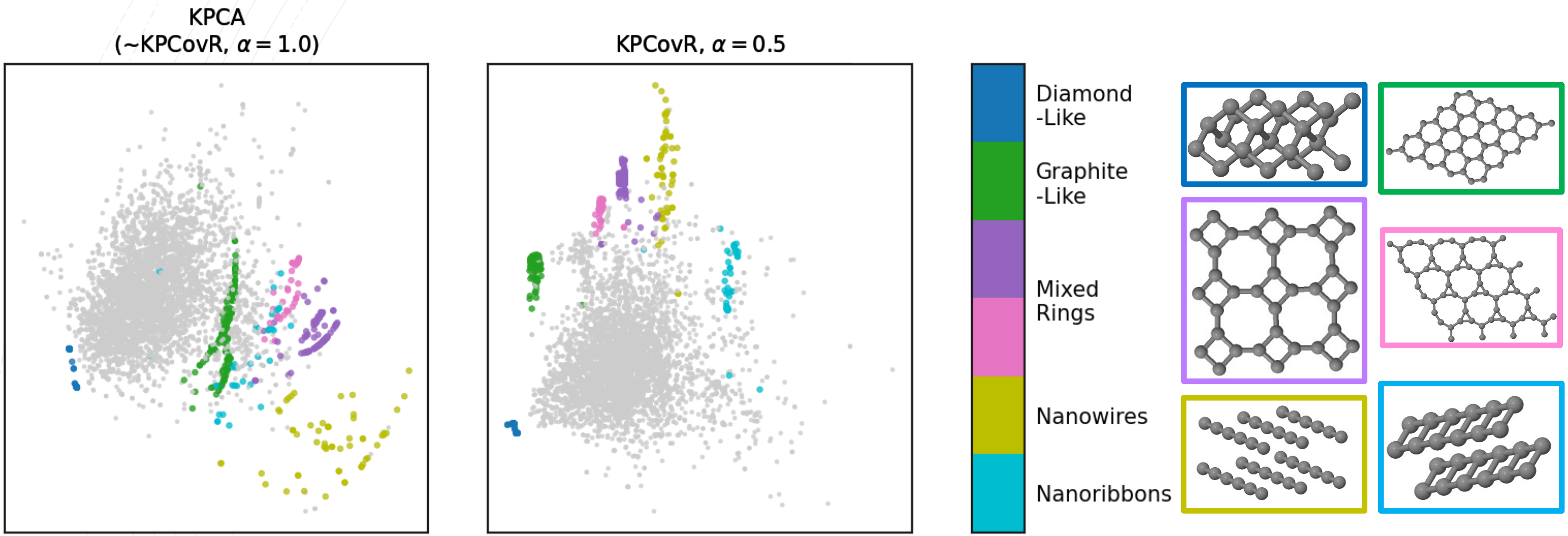

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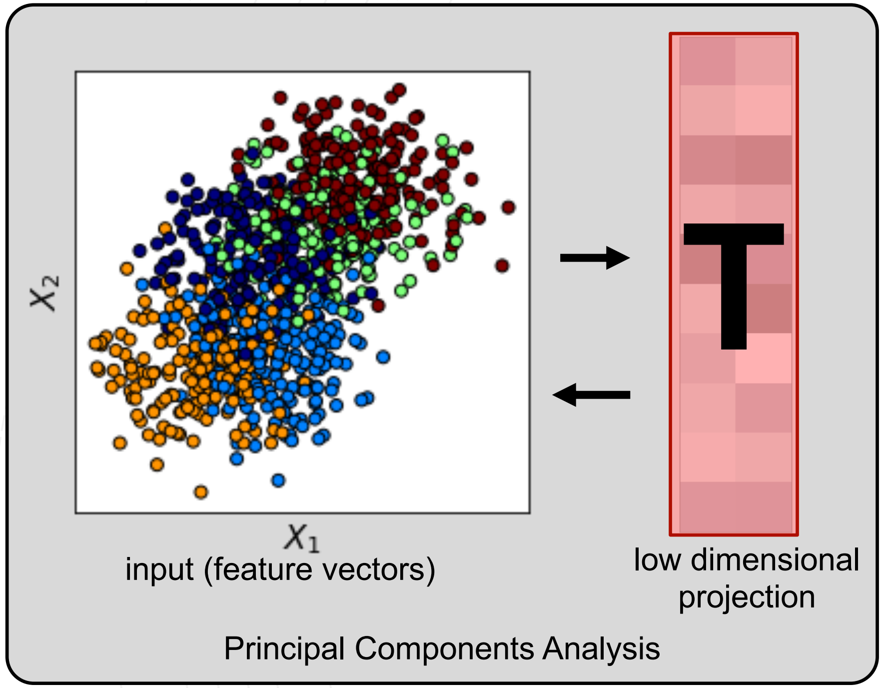
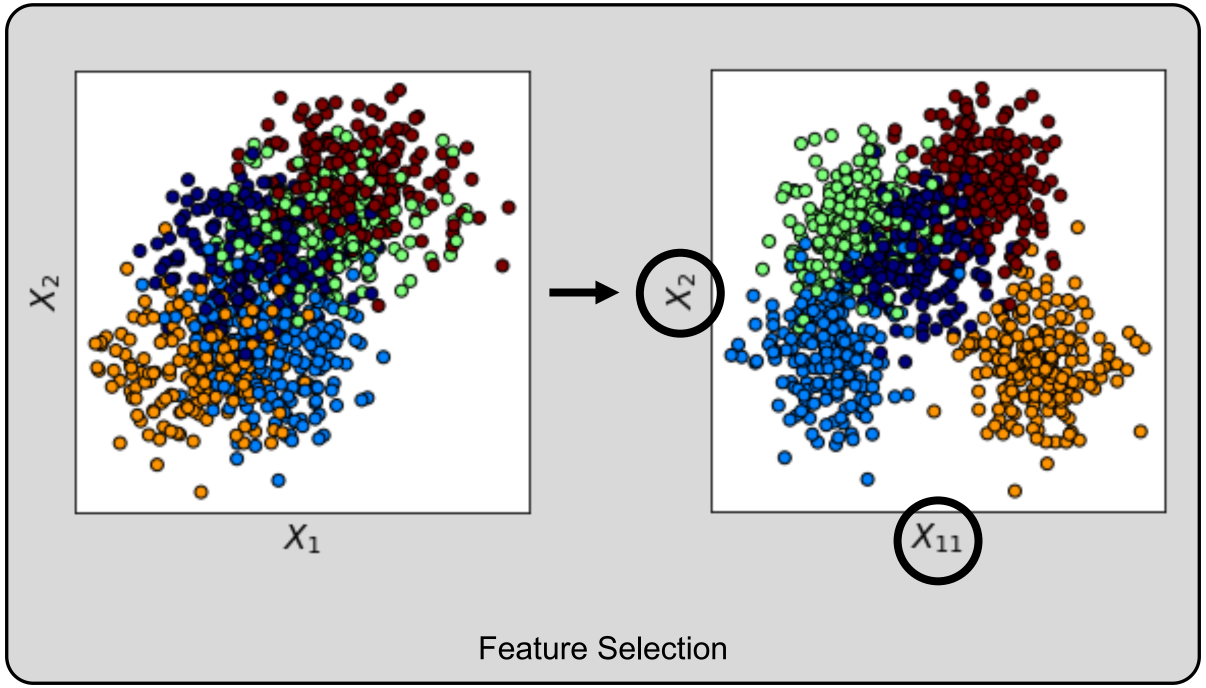
What if the features carry inherent meaning?

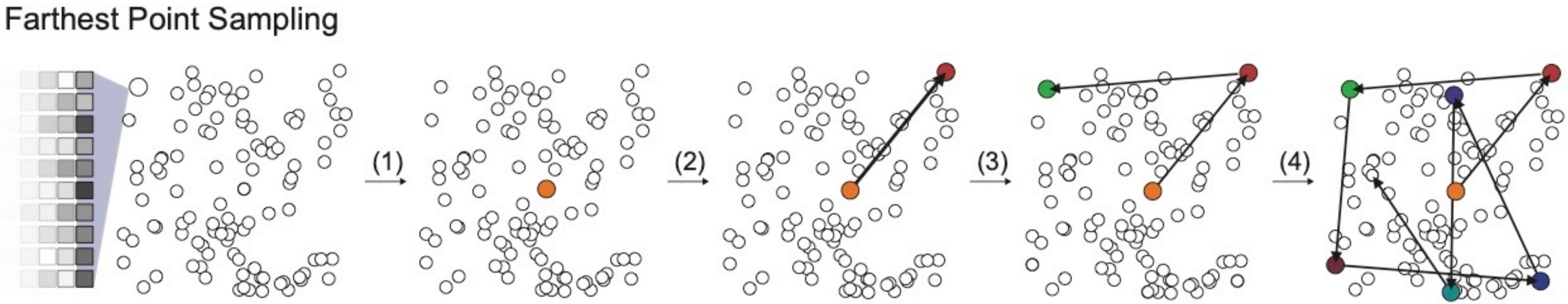
Many dimensionality reduction techniques construct a *new* set of features, but what if you want to just work with a subset of the old set?





Farthest Point Sampling (FPS)

FPS aims to select a diverse subset of features or samples that cover the greatest portion of sample or feature space.



1. Choose a first point
2. Compute distance d
3. Choose point with highest $\min(d)$ to the selected points
4. Repeat 1-3 until you have enough features!

CUR Decomposition

Traditional CUR decomposition selection aims to select "important" features or samples from the overall distribution.

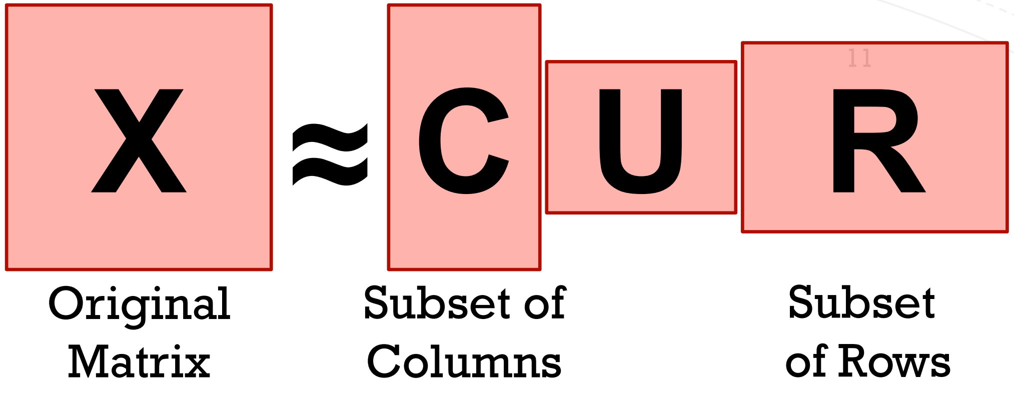
Head Canon:
"Columns und Rows" decomposition

$$X \approx C\,U\,R$$

Original Matrix

Subset of Columns

Subset of Rows



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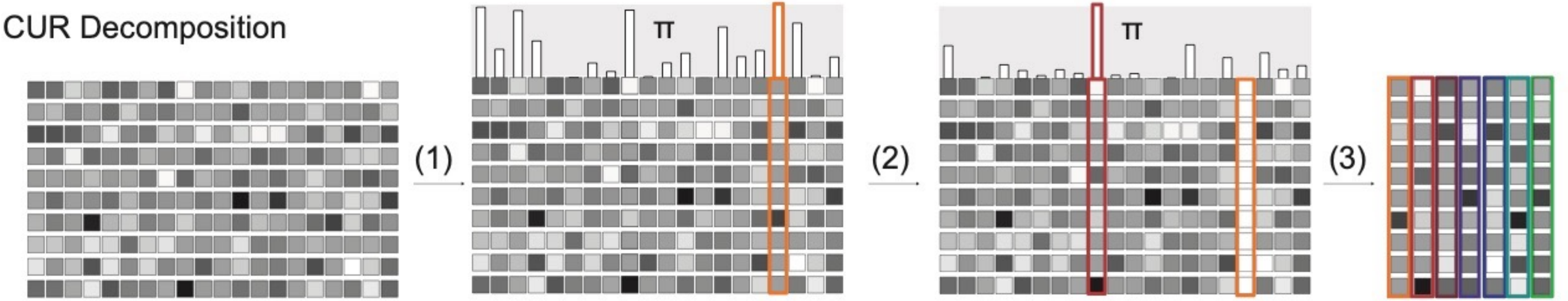

1. Compute importance score π
2. Choose column with highest π
3. Orthogonalize with respect to last chosen column.
4. Repeat 1-3 until you have enough features!

CUR Decomposition

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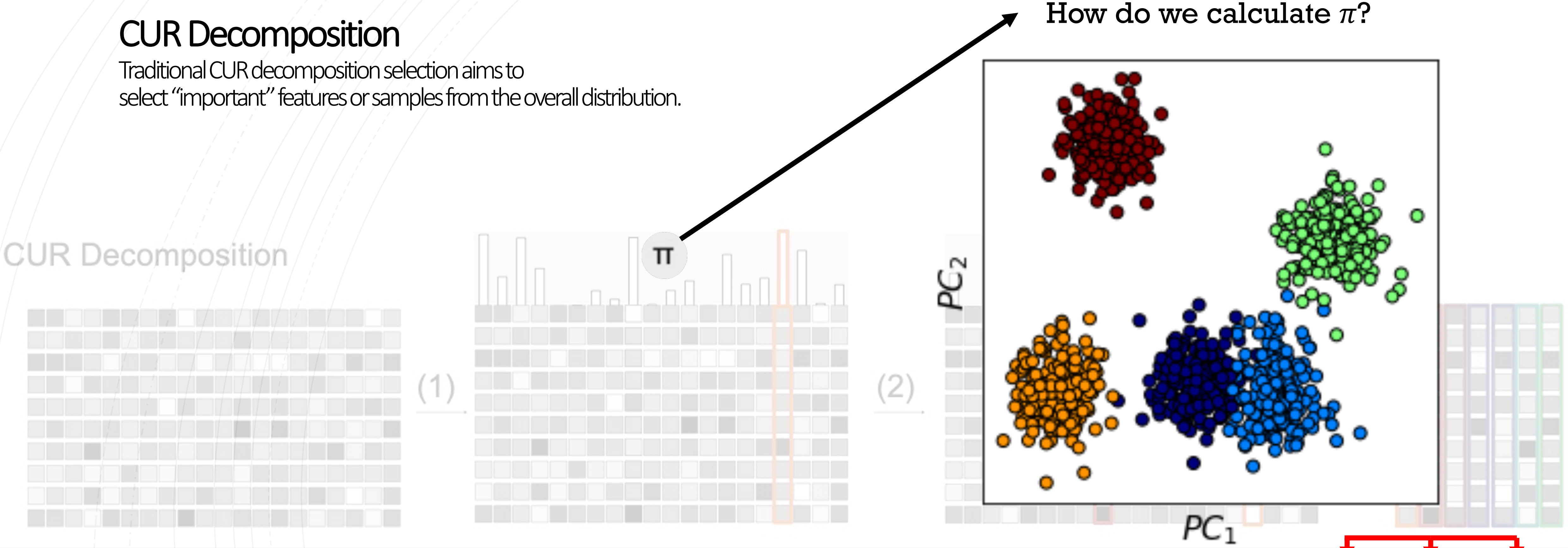
select "important" features or samples from the overall distribution.

How do we calculate π?



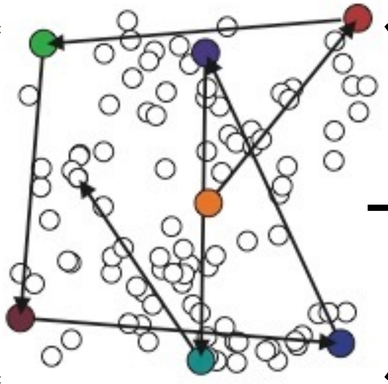
$$PC_1 = AX_1 + BX_2 + CX_3 \ldots$$

PCov-FPS and Pcov-CUR

Both FPS and CUR can be translated to PCovR space for both feature (and sample) selection.

Farthest Point Sampling (FPS)

$$d = f\Big($$



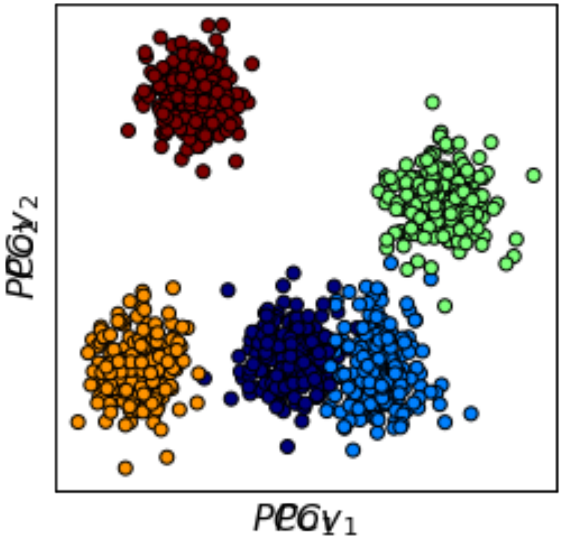
$$+$$

Contribution
to Regression
Weights

$$\Big)$$

CUR Decomposition

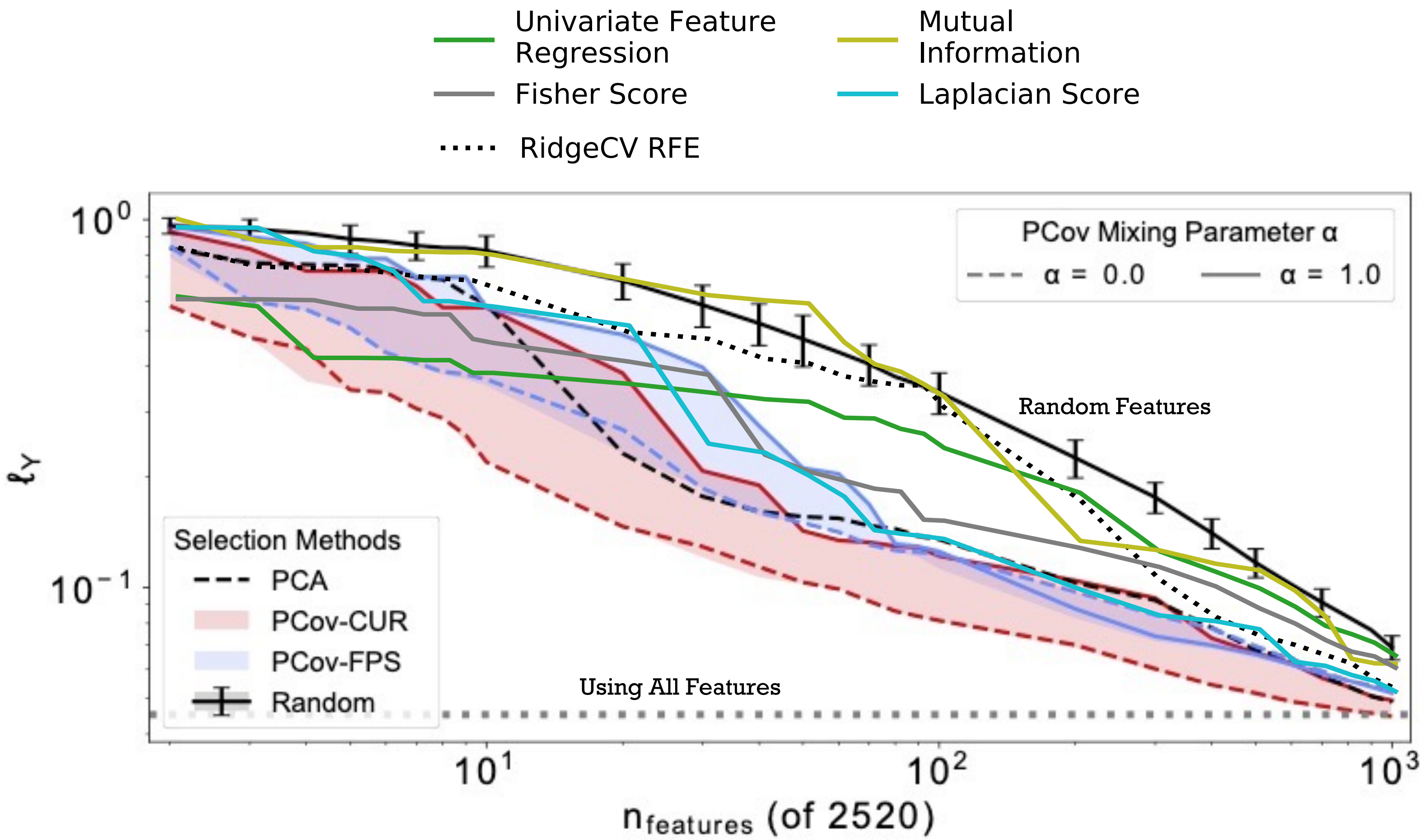
$$\pi = f\Big($$



$$\Big)$$

Linear Regression

Using PCov-style feature selection will universally out-perform common feature selection metrics available via popular packages.



Inputs: SOAP vectors for small molecules containing C + H + N + O, (9 / 1) train / test split
Target: NMR chemical shieldings in ppm
Model used: 5-fold cross-validated linear ridge regression

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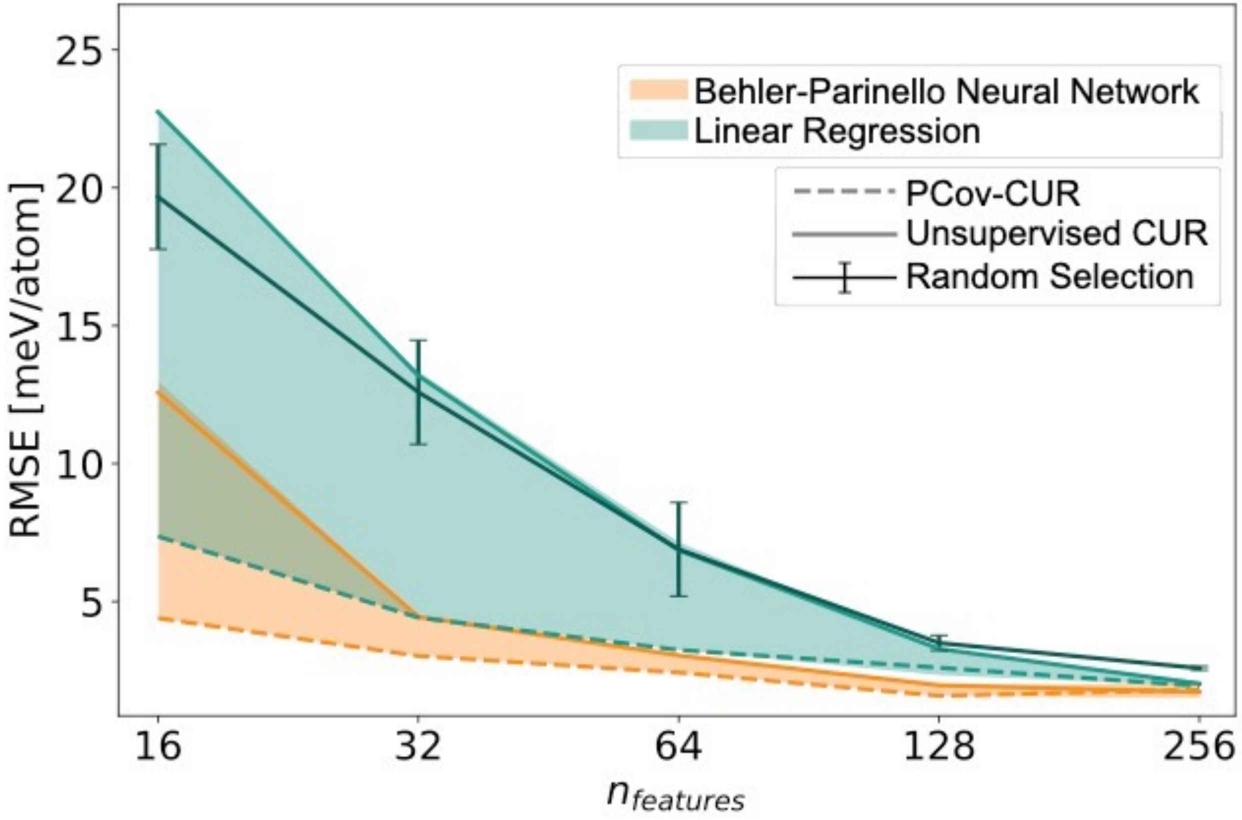
Behler-Parinello Neural Networks



Inputs: symmetry functions of benzene rings from a simulation trajectory, (7/2/1) train / validation / test split

Target: energies in [meV / atom]

Models used: 5-fold cross-validated linear ridge regression, Behler-Parinello Neural Network

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kernel-tutorials

A set of utilities and pedagogic notebooks for the use of linear and kernel methods in atomistic modeling

https://www.github.com/cosmo-epfl/kernel-tutorials/

librascal

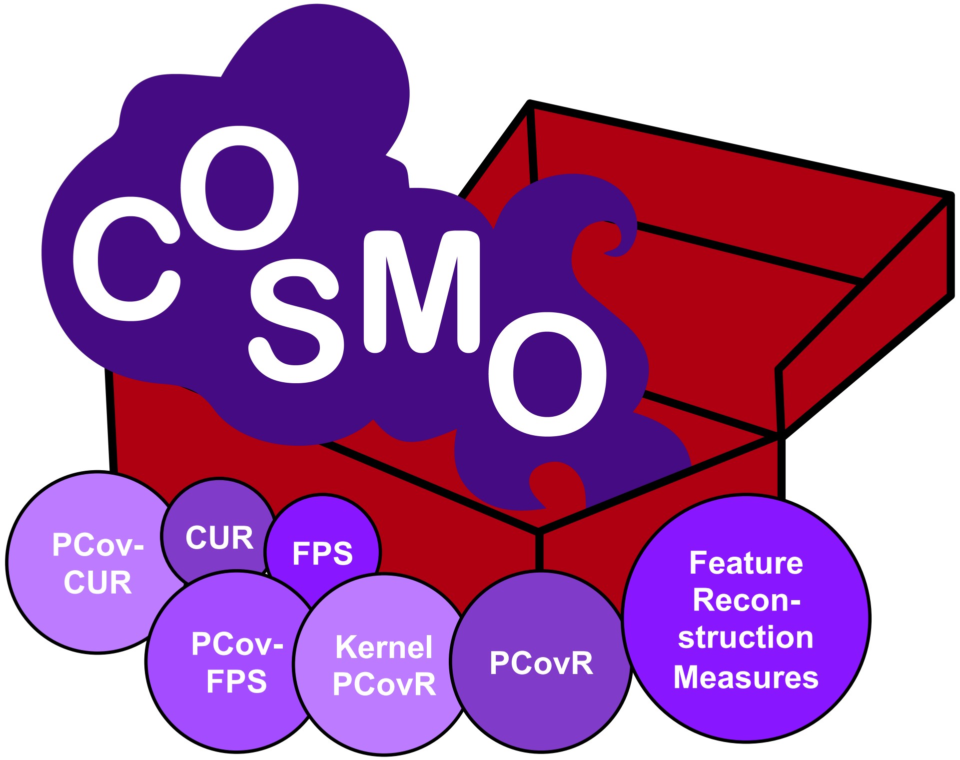
A scalable and versatile library to generate representations for atomic-scale learning

https://www.github.com/cosmo-epfl/librascal/

chemiscope

chemiscope is an interactive structure/property explorer for materials and molecules. The goal of chemiscope is to provide interactive exploration of large databases of materials and molecules and help researchers to find structure-properties correlations inside such databases.

chemiscope.org



scikit-COSMO

scikit-COSMO is a collection of scikit-learn compatible utilities that implement methods developed at COSMO.

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https://www.github.com/cosmo-epfl/scikit-cosmo/

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