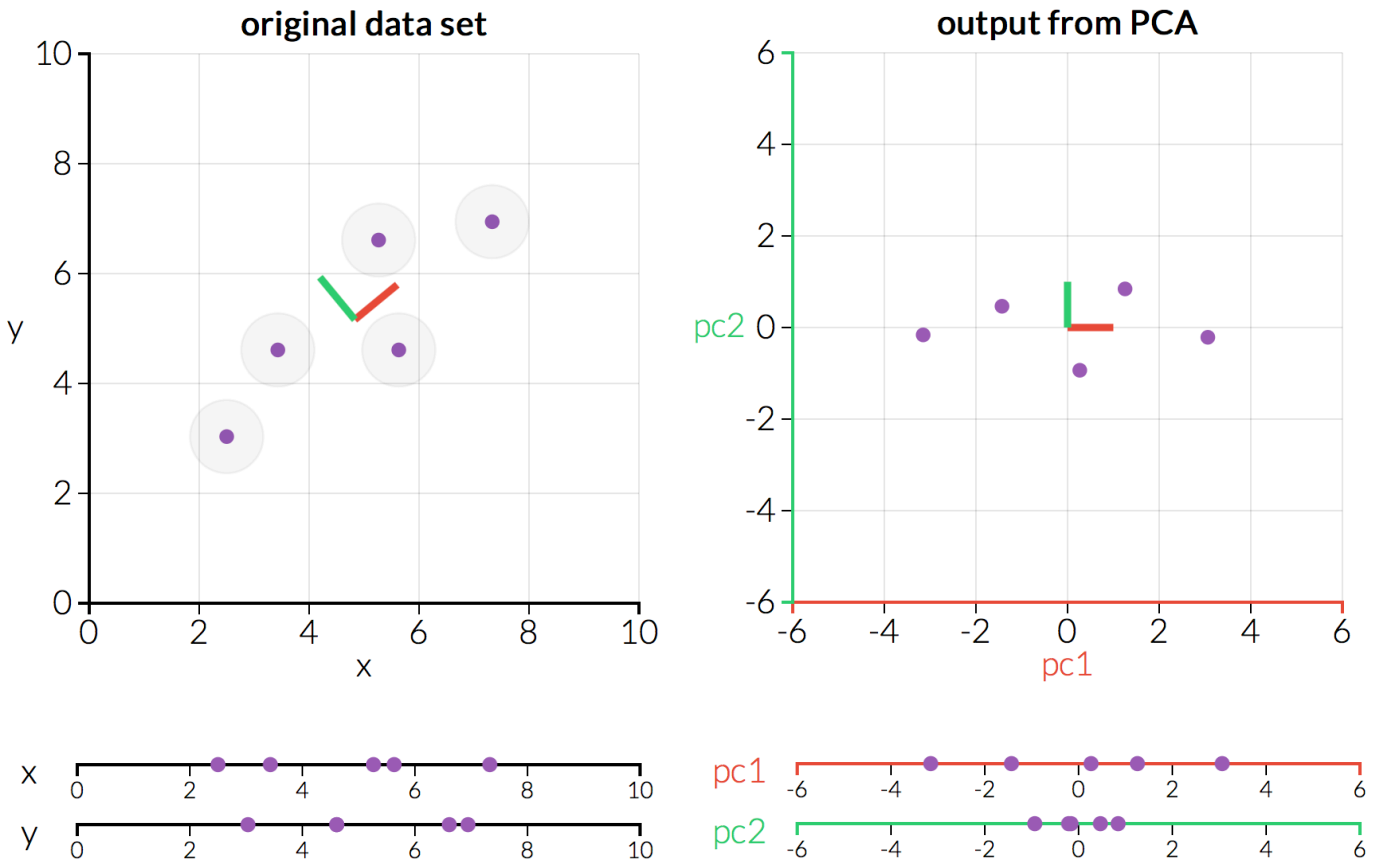
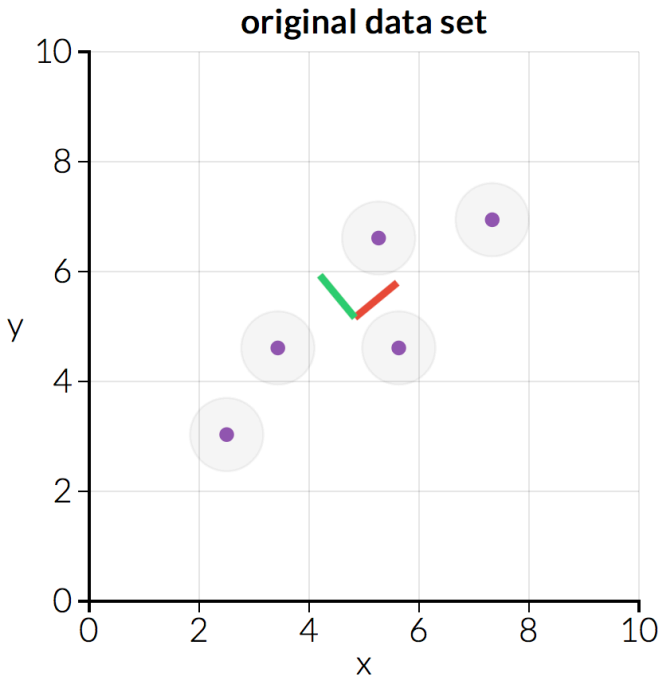
Dimensionality Reduction Using sci-kit learn

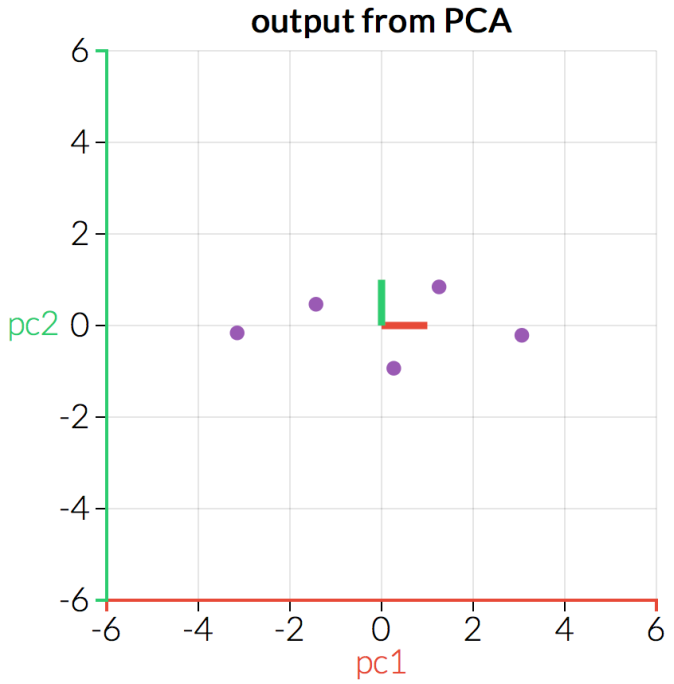
Principal Component Analysis Visualization

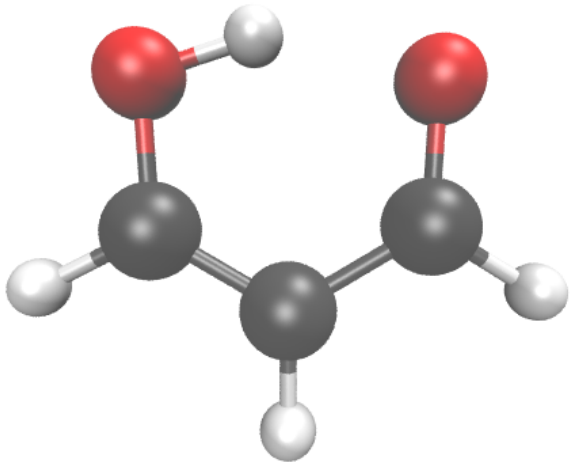


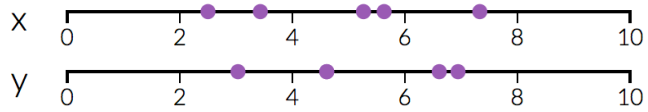
Victor Powell and Lewis Lehe, http://setosa.io/ev/principal-component-analysis/, accessed 21.03.2019

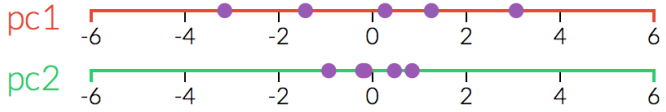
Principal Component Analysis Visualization





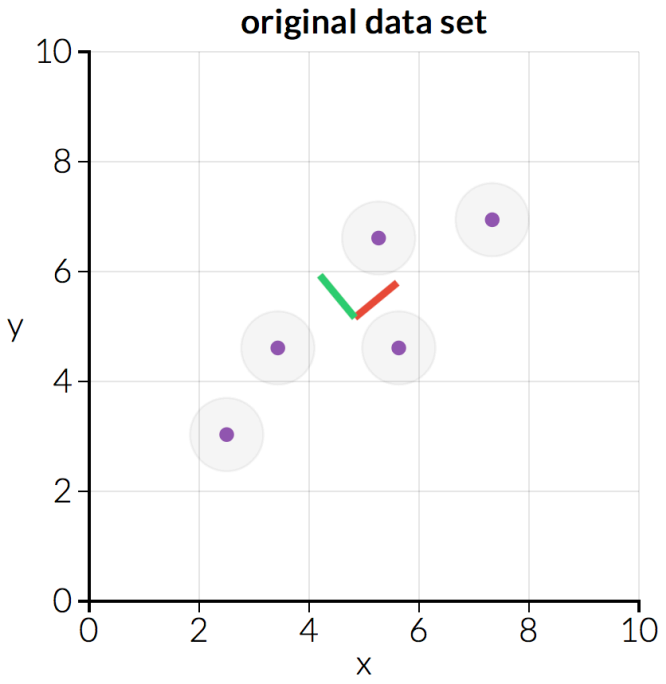


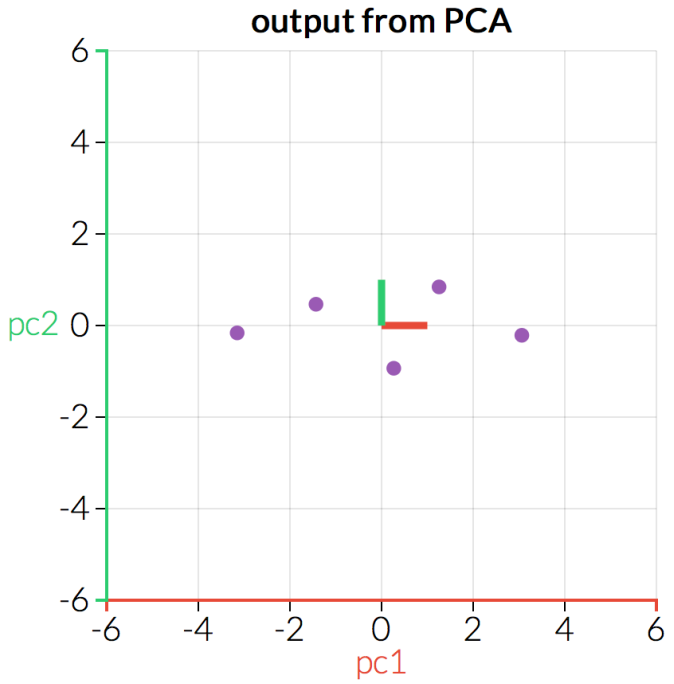


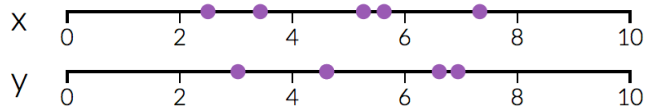


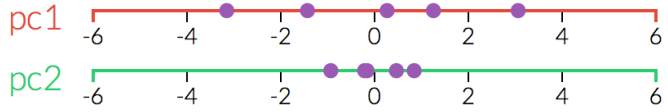
Victor Powell and Lewis Lehe, http://setosa.io/ev/principal-component-analysis/, accessed 21.03.2019

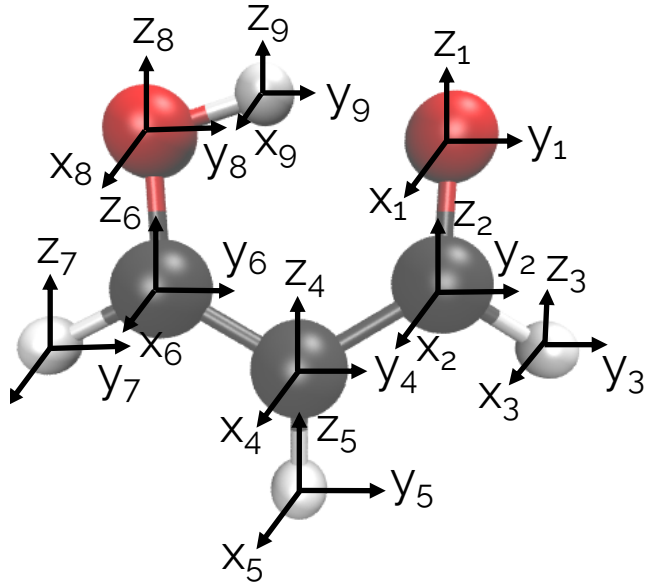
Principal Component Analysis Visualization











3N Dimensions

$(x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$

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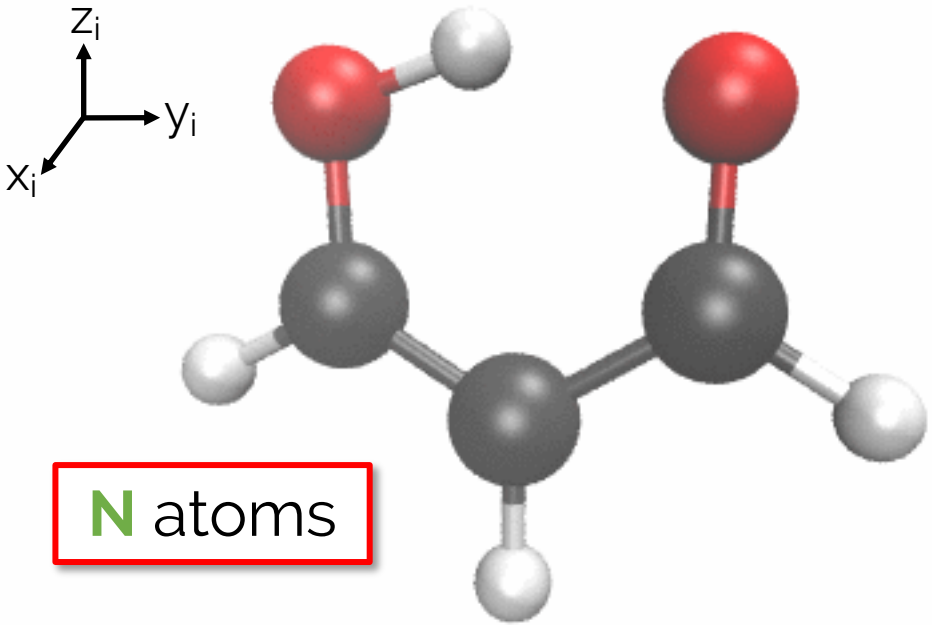
Malonaldehyde H⁺-transfer

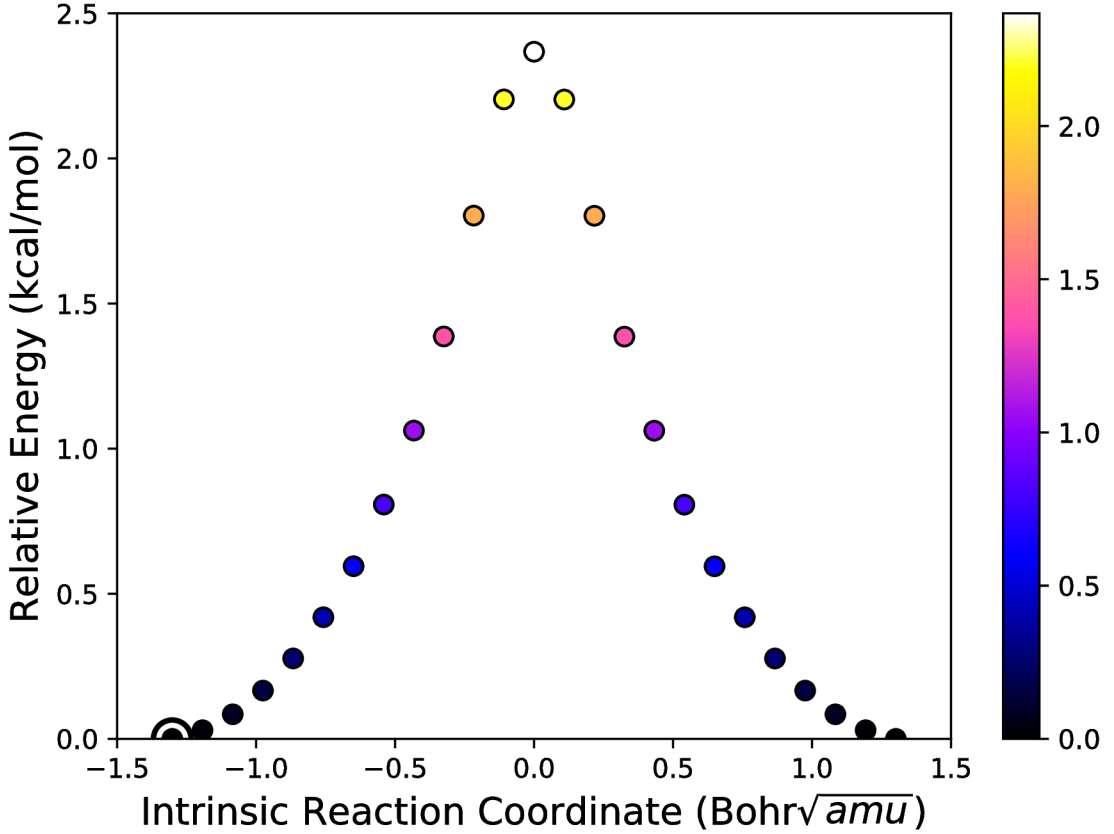
Malonaldehyde H⁺-transfer



N atoms

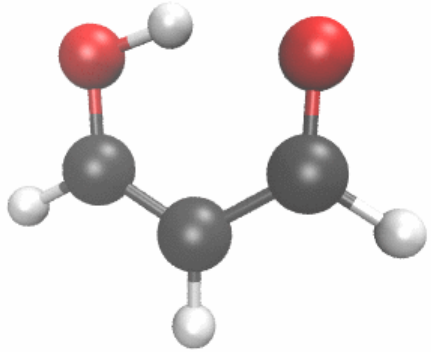
Intrinsic Reaction Coordinate (IRC)

n structures

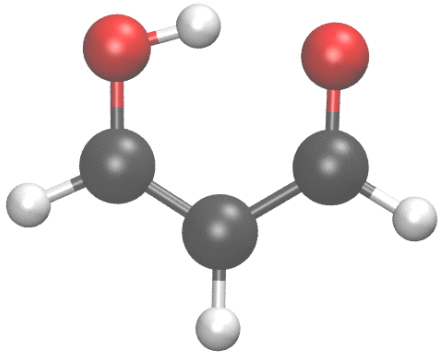


Hare, S. R.; Bratholm, L.; Glowacki, D. R.; Carpenter, B. K.; *Manuscript in progress*.

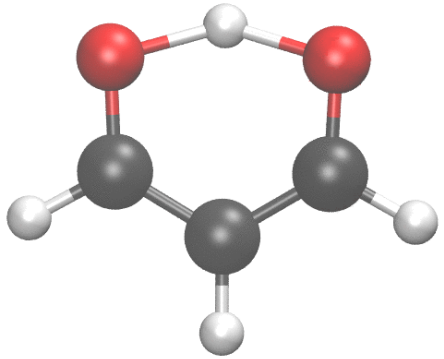
Malonaldehyde H^+-transfer



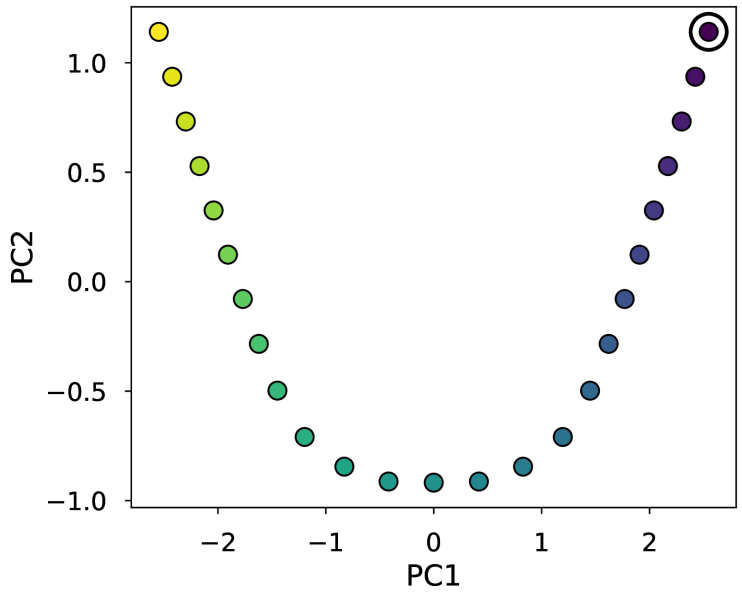
IRC

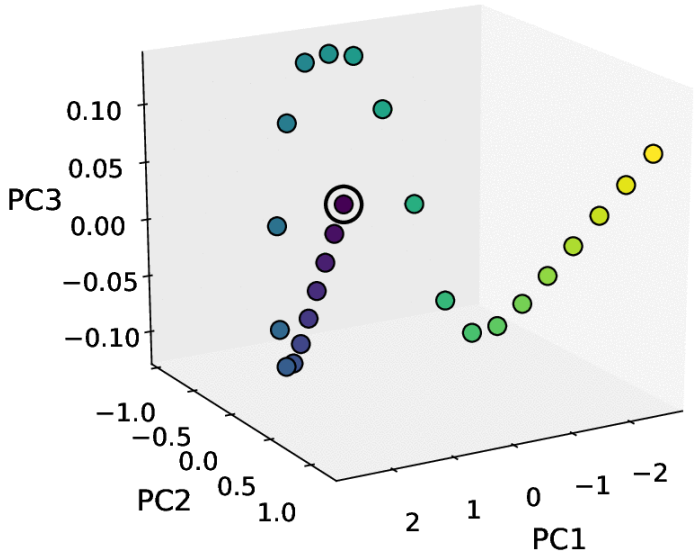


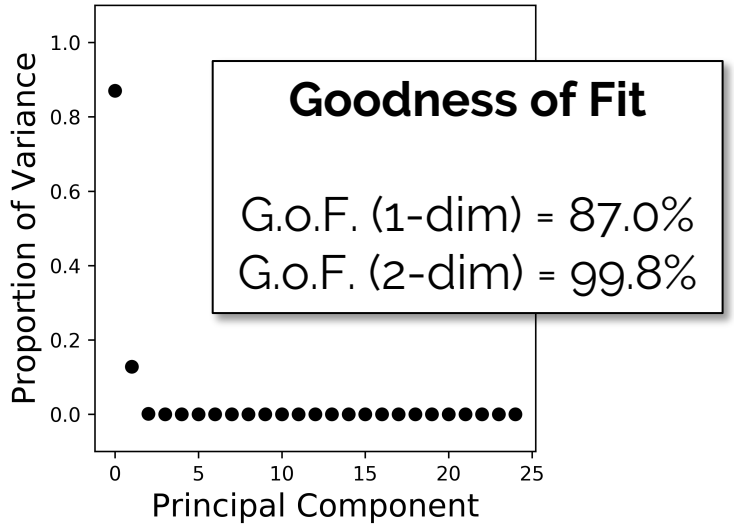
Principal Component 1 (PC1)



Principal Component 2 (PC2)



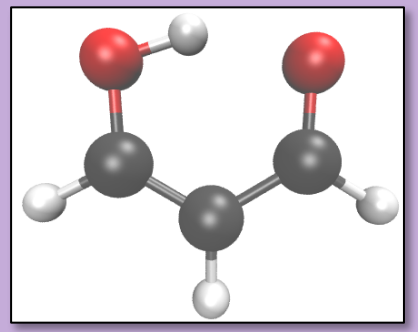




Hare, S. R.; Bratholm, L.; Glowacki, D. R.; Carpenter, B. K.; *Manuscript in progress*.

Your Task(s)

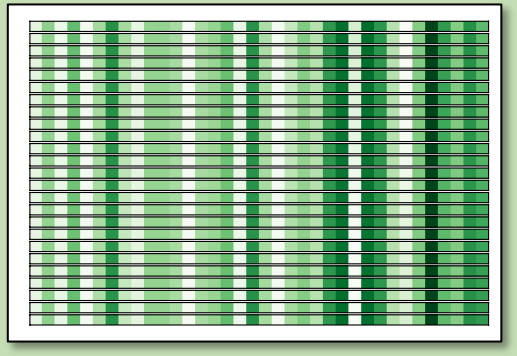
Pre-Processing



xyz file

Matrix of Data

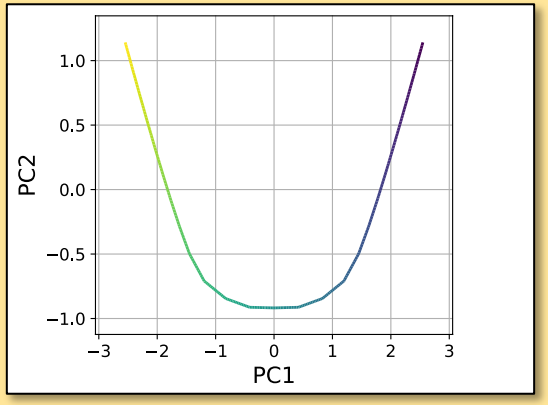
Processing



n samples x p features

PCs to Plot

Plotting



Plot(s) of top 2-3 PCs