Applications of machine learning and neural networks to data processing

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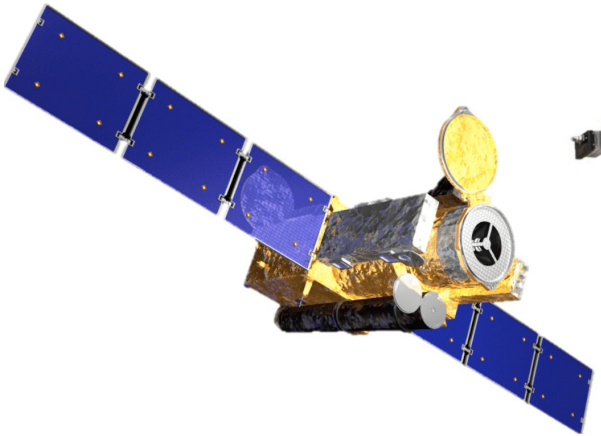
Stockholms universitet

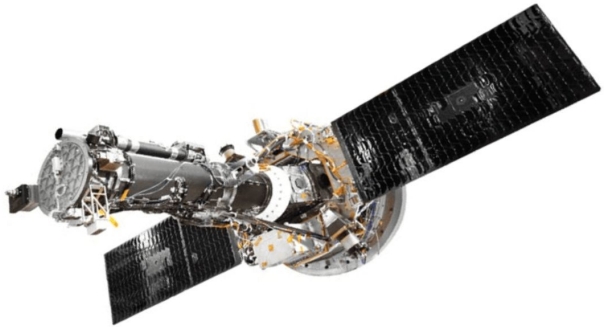
Why do we need a review?

(Pietarila et al. 2007; Viticchié & Sánchez Almeida 2011; Panos et al. 2018; Sainz Dalda et al. 2019; Bose et al. 2019; Rouppe van der Voort et al. 2021; Robustini et al. 2019; Joshi & Rouppe van der Voort 2020b; Kuckein et al. 2020; Bose et al. 2021a,b; Barczynski et al. 2021; Nóbrega-Siverio et al. 2021; Kleint & Panos 2022; Joshi et al. 2022 Asensio Ramos et al. 2007; Asensio Ramos & López Ariste 2010 Quintero Noda et al. 2015, 2016; Felipe et al 2016, Griñón-Marín 2021; Rees et al. 2000; López Ariste & Casini 2002; Skumanich & López Ariste 2002; Casini et al. 2005; Casini et al. 2009, 2013; Ruiz Cobo & Asensio Ramos (2013); Socas-Navarro et al. (2001); Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018; Bobra et al. (2015, 2016); Carroll et al. 2001, 2008; Socas-Navarro, H. 2003, 2005; Sainz Dalda et al. 2019; Milić et al. 2020; Gafeira et al. 2021; Centeno et al. 2022); Kianfar S. et al. (2019); Morosin R. et al. 2022; Skumanich & López Ariste 2002; Vishal Upendran 2020; Armstrong et al. 2021; Wang et al 2021; Deng et al 2021; Armstrong & Fletcher (2019); Ahmadzadeh et al 2019; Zhu et al. 2019; Diercke et al 2022; Felipe et al. 2019; Broock et al 2021; Pietarila et al. 2007; Viticchié & Sánchez Almeida 2011; Panos et al. 2018 2020; Sainz Dalda et al. 2019; Bose et al. 2019; Rouppe van der Voort et al. 2021; Robustini et al. 2019; Joshi & Rouppe van der Voort 2020b; Kuckein et al. 2020; Bose et al. 2021a,b; Barczynski et al. 2021; Nóbrega-Siverio et al. 2021; Kleint & Panos 2022; Joshi et al. 2022 Asensio Ramos et al. 2007; Asensio Ramos & López Ariste 2010 Quintero Noda et al. 2015, 2016; Felipe et al 2016, Griñón-Marín 2021; Rees et al. 2000; López Ariste & Casini 2002; Skumanich & López Ariste 2002; Casini et al. 2005; Casini et al. 2009, 2013; Ruiz Cobo & Asensio Ramos (2013); Socas-Navarro et al. (2001); Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018; Bobra et al. (2015, 2016); Carroll et al. 2001, 2008; Socas-Navarro, H. 2003, 2005; Szenicer et al 2019; Lim et al 2021; Salvatelli et al 2022; *Yes, your paper should be also around here*; Milić et al. 2020; Gafeira et al. 2021; Centeno et al. 2022; Kianfar S. et al. (2019); Morosin R. et al. (2022); Skumanich & López Ariste 2002; Asensio Ramos 2018, 2021; Armstrong et al. 2021; Wang et al 2021; Deng et al 2021; Armstrong & Fletcher (2019); Ahmadzadeh et al 2019; Zhu et al. 2019; Diercke et al 2022; Felipe et al. 2019; Broock et al 2021; Pietarila et al. 2007; Viticchié & Sánchez Almeida 2011; Panos et al. 2018; Sainz Dalda et al. 2019; Bose et al. 2019; Rouppe van der Voort et al. 2021; Robustini et al. 2019; Joshi & Rouppe van der Voort 2020b; Kuckein et al. 2020; Bose et al. 2021a,b; Barczynski et al. 2021; Nóbrega-Siverio et al. 2021; Kleint & Panos 2022; Joshi et al. 2022 Asensio Ramos et al. 2007; Thoen Faber 2022; Quintero Noda et al. 2015, 2016; Felipe et al 2016, Griñón-Marín 2021; Rees et al. 2000; López Ariste & Casini 2002; Skumanich & López Ariste 2002; Casini et al. 2005; Casini et al. 2009, 2013; Ruiz Cobo & Asensio Ramos 2013; Socas-Navarro et al. 2001; Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018; Bobra et al. (2015, 2016); Carroll et al. 2001, 2008; Socas-Navarro, H. 2003, 2005; Sainz Dalda et al. 2019; Milić et al. 2020; Gafeira et al. 2021; Centeno et al. 2022); Kianfar S. et al. (2019); Morosin R. et al. (2022); Skumanich & López Ariste 2002; Vishal Upendran 2020; Armstrong et al. 2021; Wang et al 2021; Deng et al 2021; Armstrong & Fletcher (2019); Ahmadzadeh et al 2019; Zhu et al. 2019; Diercke et al 2022; Felipe et al. 2019; Broock et al 2021; Pietarila et al. 2007; Viticchié & Sánchez Almeida 2011; Panos et al. 2018; Sainz Dalda et al. 2019; Bose et al. 2019; Rouppe van der Voort et al. 2021; Robustini et al. 2019; Joshi & Rouppe van der Voort 2020b; Kuckein et al. 2020; Bose et al. 2021a,b; Barczynski et al. 2021; Nóbrega-Siverio et al. 2021; Kleint & Panos 2022; Joshi et al. 2022 Asensio Ramos et al. 2007; Asensio Ramos & López Ariste 2010; Quintero Noda et al. 2015, 2016; Felipe et al 2016, Griñón-Marín 2021; Rees et al. 2000; López Ariste & Casini 2002; Skumanich & López Ariste 2002; Thoen Faber 2022; Casini et al. 2005; Casini et al. 2009, 2013; Ruiz Cobo & Asensio Ramos (2013); Socas-Navarro et al. (2001); Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018; Bobra et al. (2015, 2016); Carroll et al. 2001, 2008; Socas-Navarro, H. 2003, 2005 2009; Sainz Dalda et al. 2019; Milić et al. 2020; Gafeira et al. 2021; Centeno et al. 2022); Kianfar S. et al. (2019); Morosin R. et al. (2022); Skumanich & López Ariste 2002; Asensio Ramos 2018,2021; Armstrong et al. 2021; Wang et al 2021; Deng et al 2021; Armstrong & Fletcher 2019, 2021; Ahmadzadeh et al 2019; Zhu et al. 2019; Diercke et al 2022; Szenicer et al 2019; Lim et al 2021; Salvatelli et al 2022)

¿Big Data?



Hinode/SOT (2006-now) ~ 35 TB*
*Level 1 (FG) + 1&2 (SP)



IRIS (2013-now) ~ 61 TB*
*Level 2

DKIST, EST, SST ~ TB/h/instr

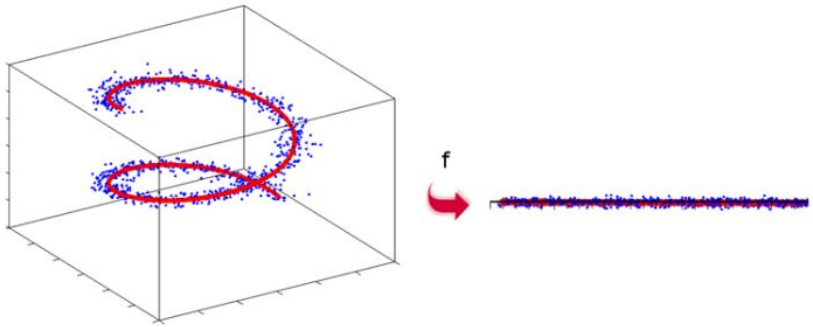
Numbers courtesy of Bart De Pontieu, Marc DeRosa, Ryan Timmons

Exploration and dimensionality reduction

Typical questions of someone that recently got a big dataset:

- How diverse vs big is my dataset?

- How many of these features are actually really **informative** or contain just **redundant** information?



Original data space

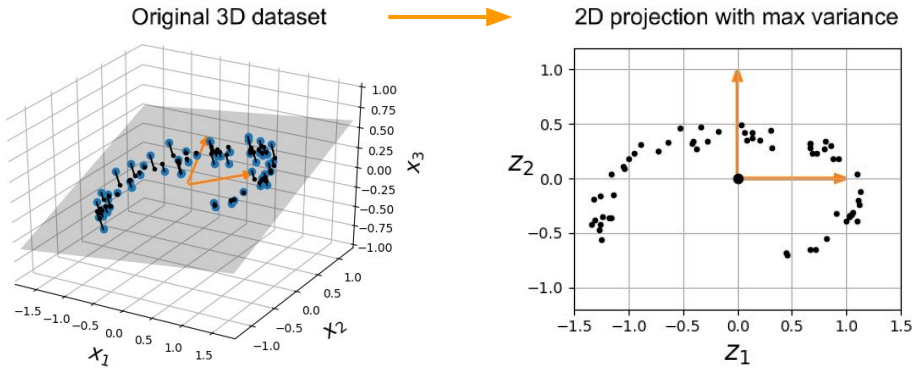
Transformed space

Dimensionality reduction: Principal Component Analysis

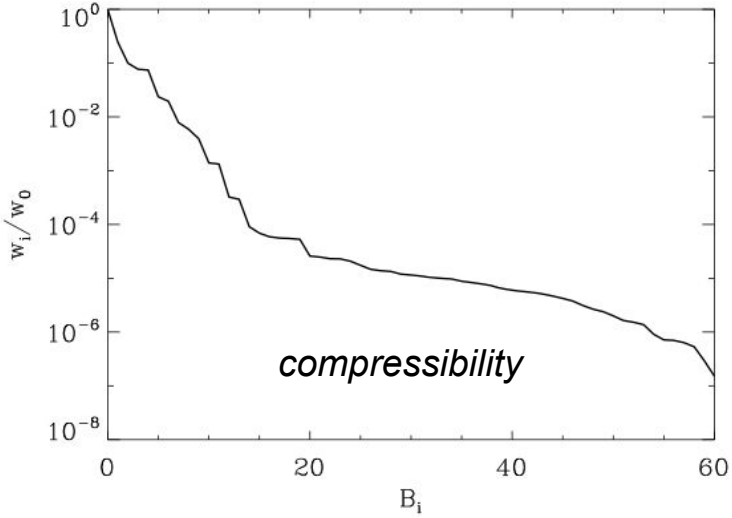
What is the basic idea behind PCA?

1.- Find the “principal components” basis

2.- Project the data into a truncated version of it.



Why is it useful in solar observations?

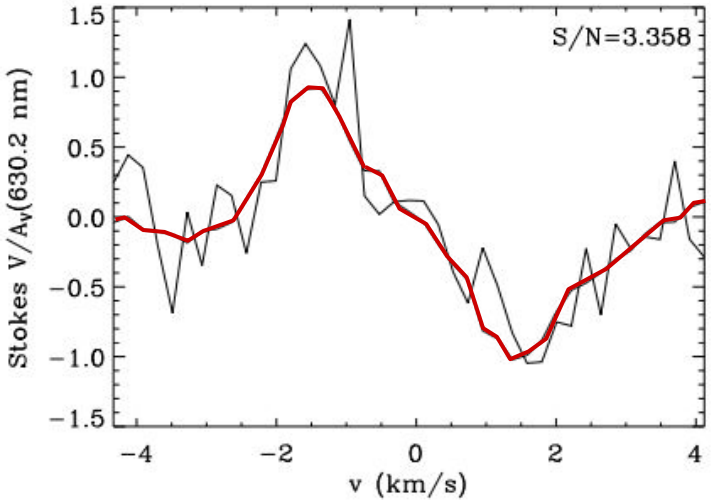


Martínez González et al. (2008a)

(e.g. Asensio Ramos et al. 2007; Asensio Ramos & López Ariste 2010)

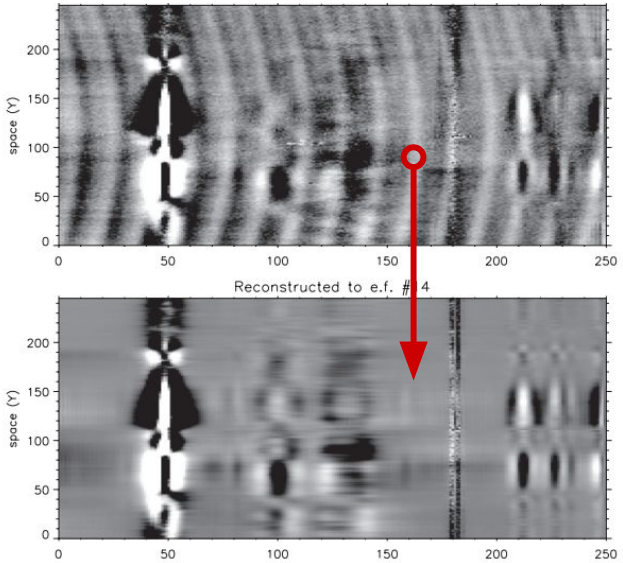
Dimensionality reduction: PCA applications

Denoising



Martínez González et al. (2008a,b)

Removal of fringes

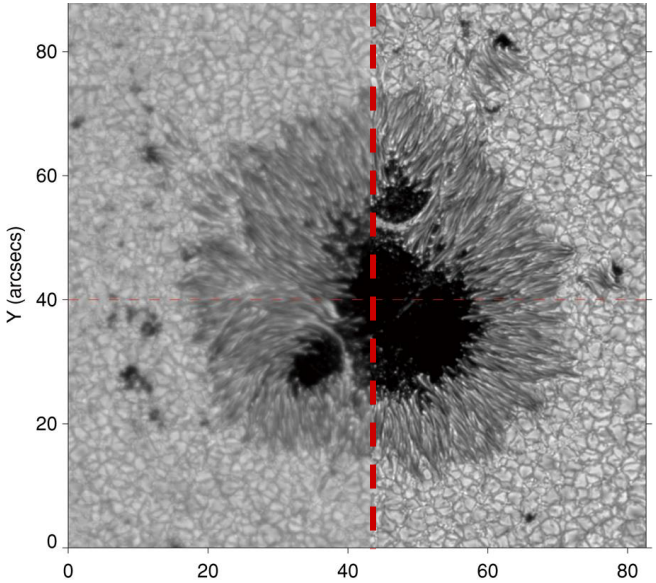


Casini et al. (2012, 2021)

(e.g. Asensio Ramos et al. 2007; Asensio Ramos & López Ariste 2010; Paletou 2012; Pastor Yabar et al. 2018; Trelles Arjona et al. 2021)

Dimensionality reduction: PCA applications

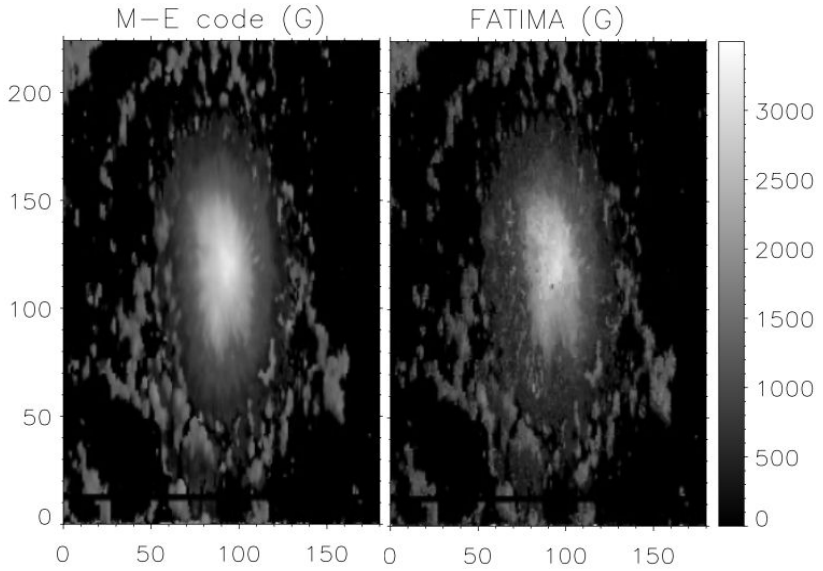
PCA deconvolution



Ruiz Cobo & Asensio Ramos (2013)

(e.g. Quintero Noda et al. 2015, 2016; Felipe et al. 2016, Griñón-Marín 2021)

PCA inversion



Socas-Navarro et al. (2001)

(e.g. Rees et al. 2000; López Ariste & Casini 2002; Skumanich & López Ariste 2002; Casini et al. 2005; Casini et al. 2009, 2013; Sainz Dalda et al. 2019)

Finding patterns

Once we have processed our dataset …

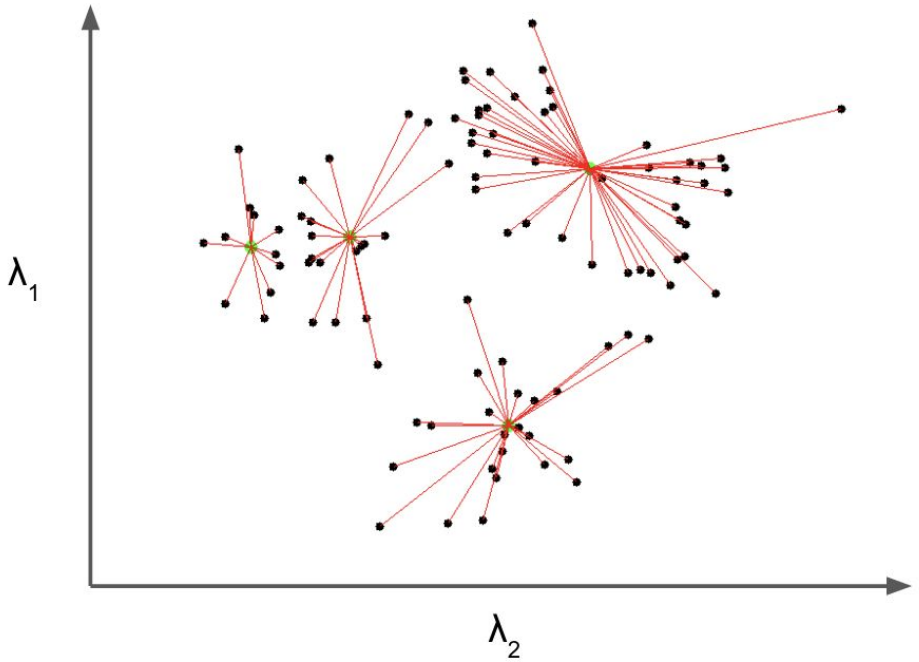
- Can I find a way to distinguish “groups” of similar properties?
- The conclusions will be the same for all the examples within the group!
- Where are all these “groups” located in the solar surface?

Clustering: K-means algorithm

1.- Define the K clusters and draw the **centroids**

2.- Assign each point to the closest centroid (Euclidean **distance**)

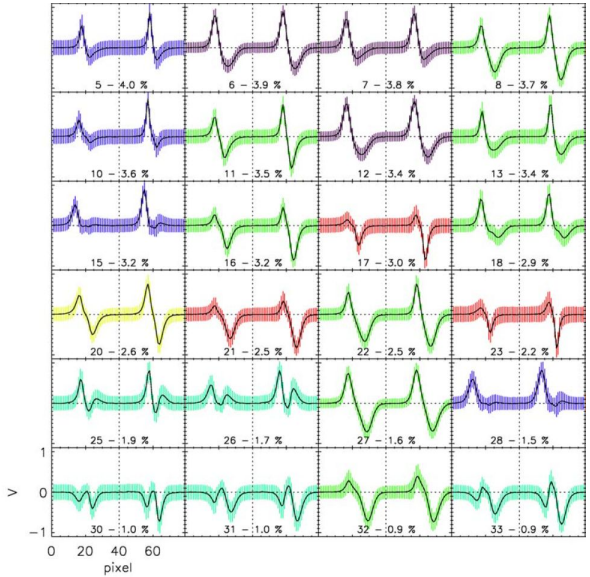
3.- The centroids are updated as the average of their cluster



(e.g., Pietarila et al. 2007; Viticchié & Sánchez Almeida 2011; Panos et al. 2018; Sainz Dalda et al. 2019; Bose et al. 2019; Rouppe van der Voort et al. 2021; Robustini et al. 2019; Joshi & Rouppe van der Voort 2020b; Kuckein et al. 2020; Bose et al. 2021a,b; Barczynski et al. 2021; Nóbrega-Siverio et al. 2021; Kleint & Panos 2022; Joshi et al. 2022; Thoen Faber 2022).

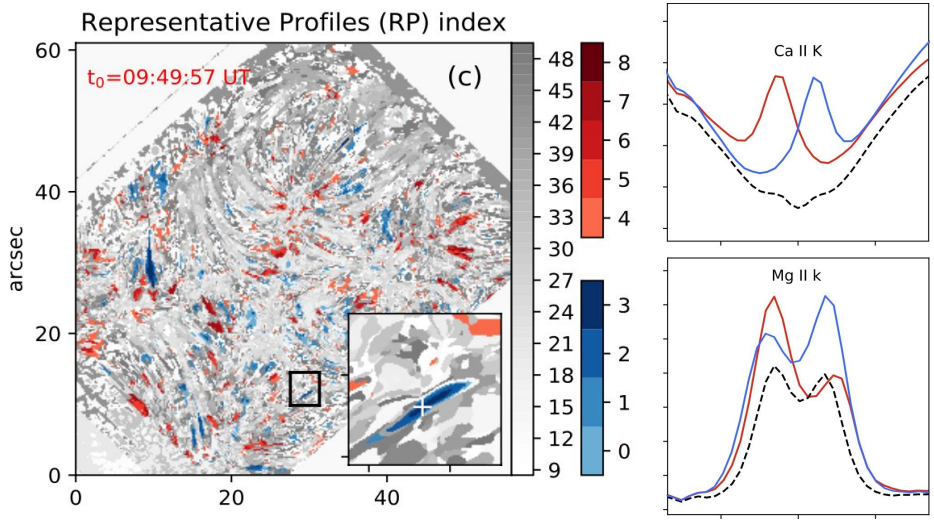
K-means applications

QS magnetic field



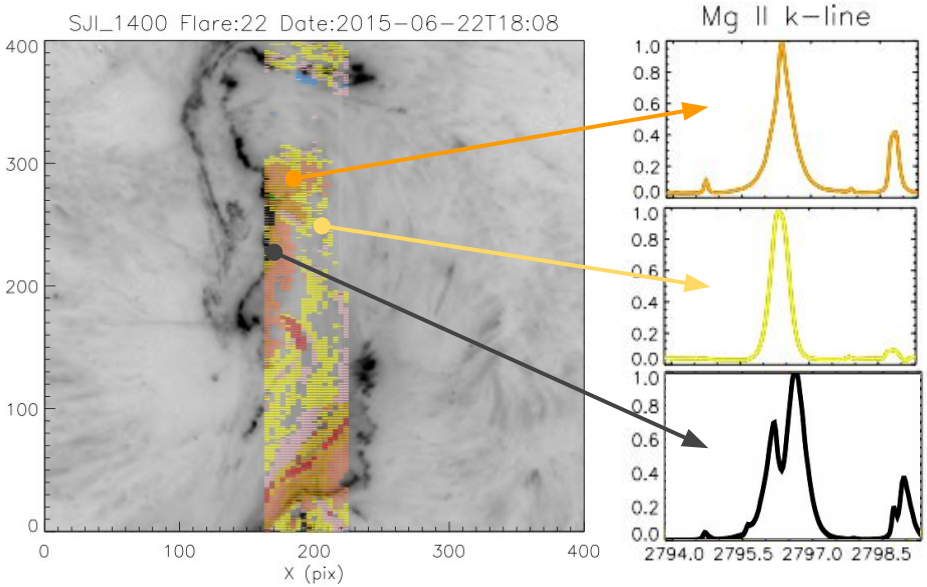
Viticchié & Sánchez Almeida (2011)

Type-II Spicules

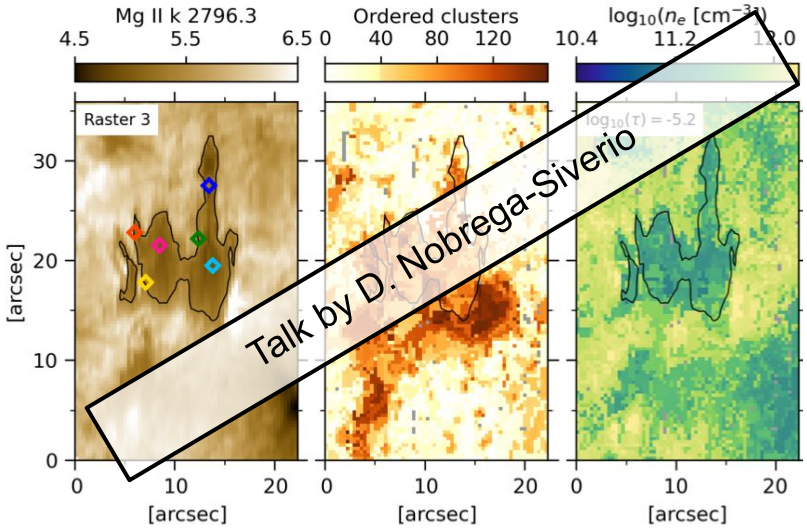


Bose et al. (2019, 2021a,b)

K-means applications



Brandon Panos et al. (2018)



Nóbrega-Siverio et al. (2021)

(e.g. Magnus Woods et al. 2021)

PCA and k-means are not the only ones

Dimensionality reduction

- Feature selection
- Principal Component Analysis (PCA)
- Non-negative matrix factorization (NMF)
- Linear discriminant analysis (LDA)
- Generalized discriminant analysis (GDA)
- Missing Values Ratio
- Low Variance Filter
- High Correlation Filter
- Backward Feature Elimination
- Forward Feature Construction
- t-SNE (T-distributed stochastic neighbour embedding)

Clustering techniques

- Affinity Propagation
- Agglomerative Hierarchical Clustering
- BIRCH (Balanced Iterative Reducing and Clustering using Hierarchies)
- DBSCAN (Density-Based Spatial Clustering of Applications with Noise)
- Gaussian Mixture Models (GMM)
- K-Means
- Mean Shift Clustering
- Mini-Batch K-Means
- OPTICS
- Spectral Clustering

Classification and prediction

Once you know the interesting part in our dataset …

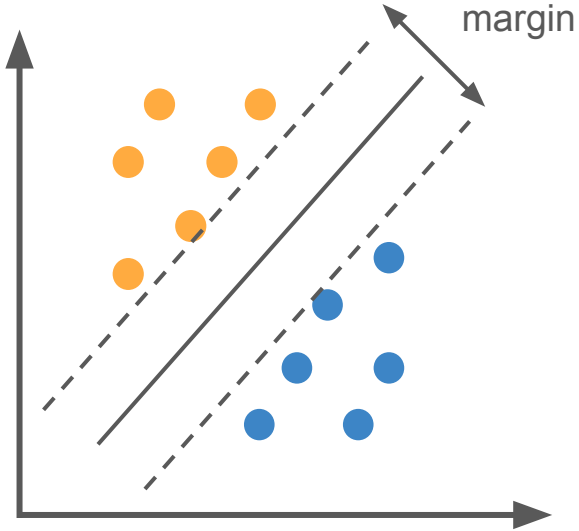
- Can we find a recipe that links our **data** with some **properties**?
  - they can come from different sources
  - just very computationally expensive
  - very difficult to manually find a way

- Can it be general enough to be applied to future data?

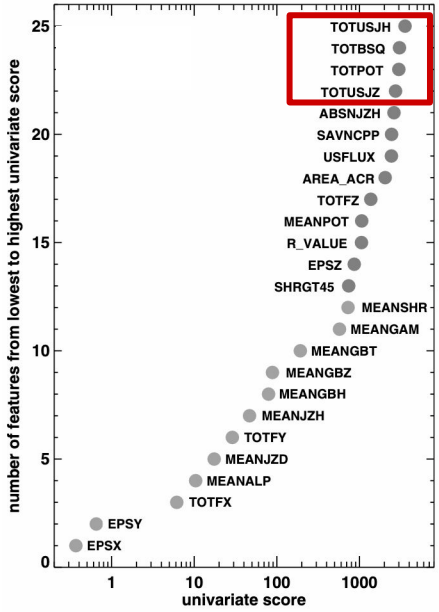
- Even more important, can we learn something from it?

Classification and prediction

Support Vector Machines



Flare prediction

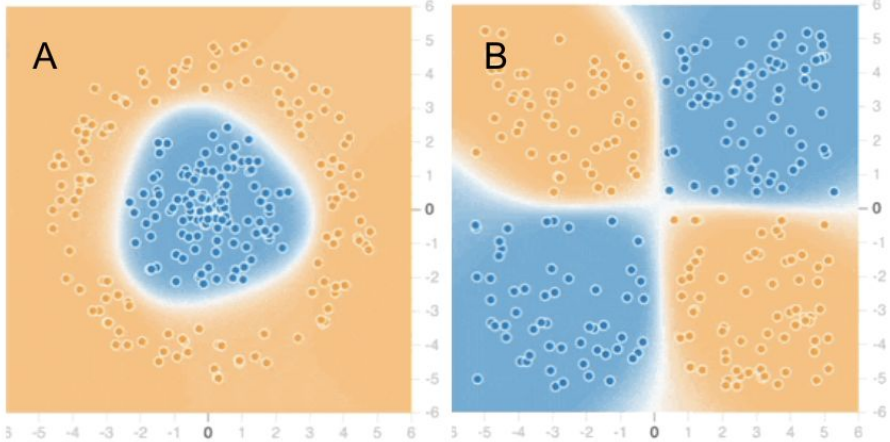


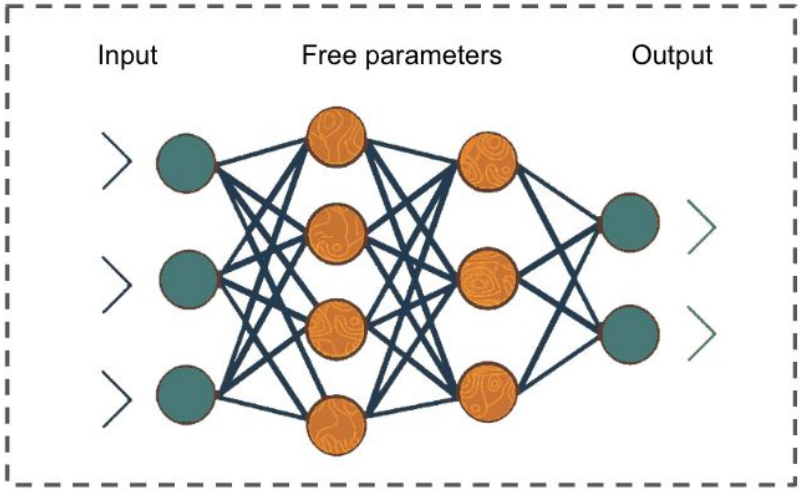
Bobra et al. (2015, 2016)

(e.g. Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018)

Nonlinear modeling → Neural networks

What happens if this relation that we try to model is very non-linear?

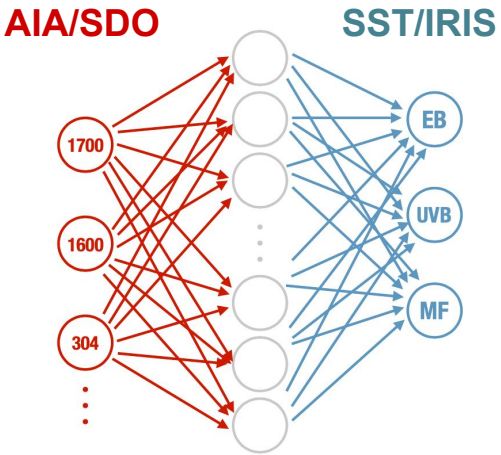


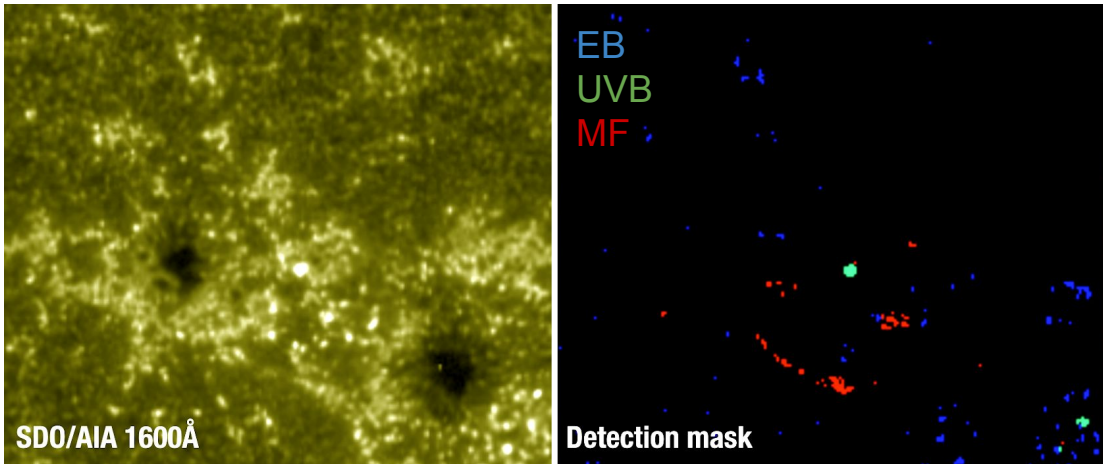


$$o_i = f\left(\Sigma_j x_j \cdot w_j + b_j\right)$$

Neural networks for classification

Detection of reconnection events … in larger FOVs and longer time periods

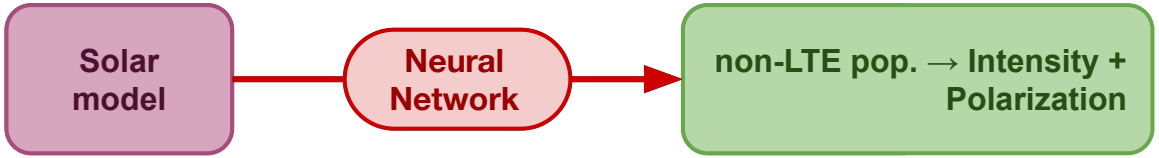




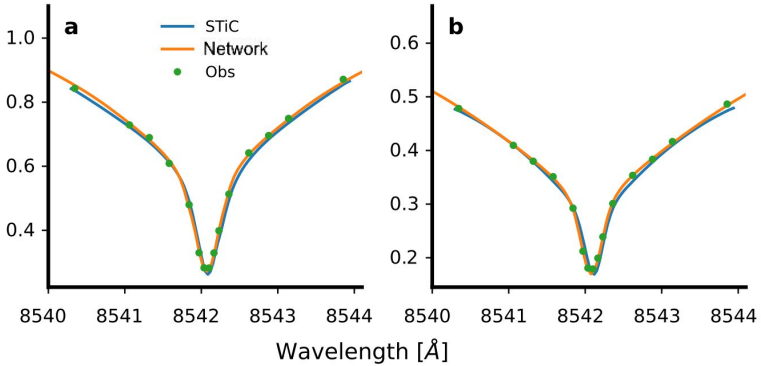
Vissers et al. (in prep)

(e.g. Yuan et al. 2010; Nishizuka et al. 2017; Florios et al. 2018; Panos et al. 2018; Huwyler et al. 2022)

NLTE Radiative transfer calculations

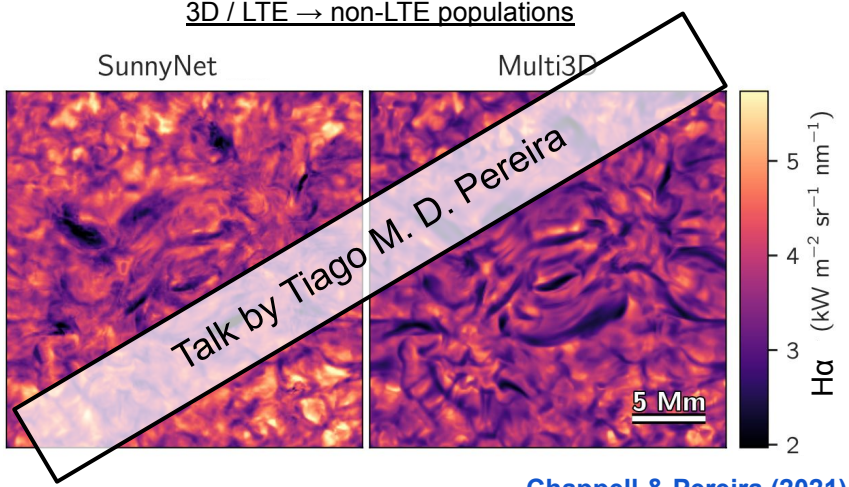


1D / departure coefficients



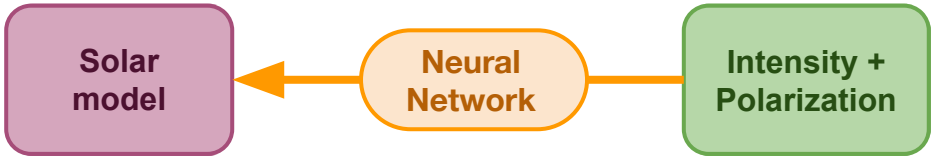
Vicente Arévalo et al. (2021)

3D / LTE → non-LTE populations

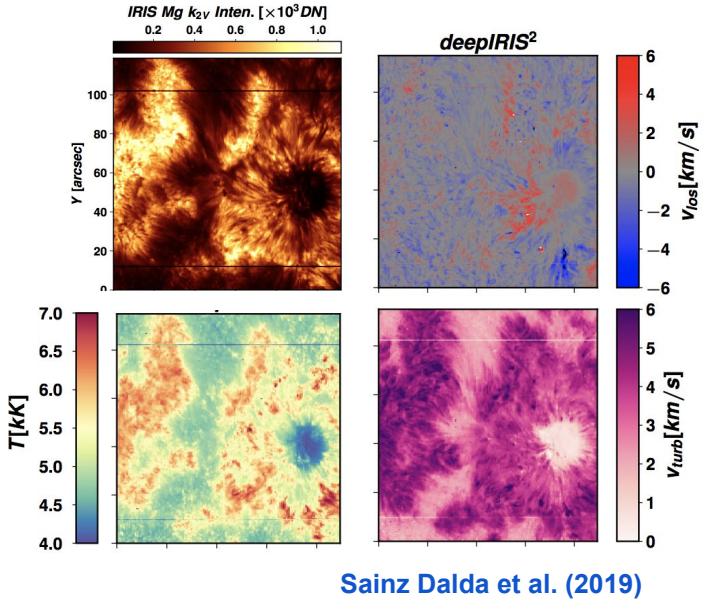


Chappell & Pereira (2021)

Spectropolarimetric inversions



Synthesis + Inversions ~ 10^3 - 10^6 faster

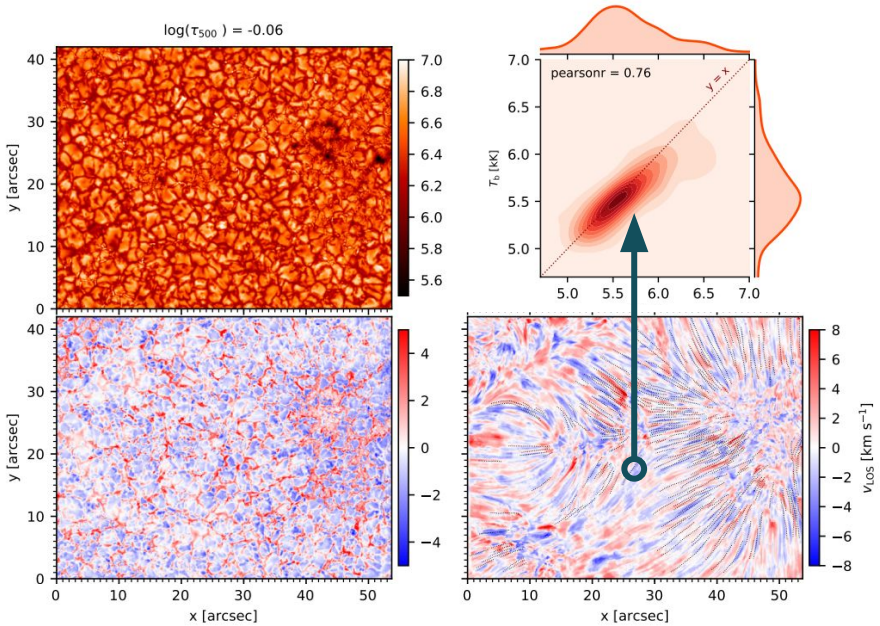


Sainz Dalda et al. (2019)

(e.g. Carroll et al. 2001, 2008; Socas-Navarro, H. 2003, 2005; Sainz Dalda et al. 2019; Milić et al. 2020; Gafeira et al. 2021; Centeno et al. 2022)

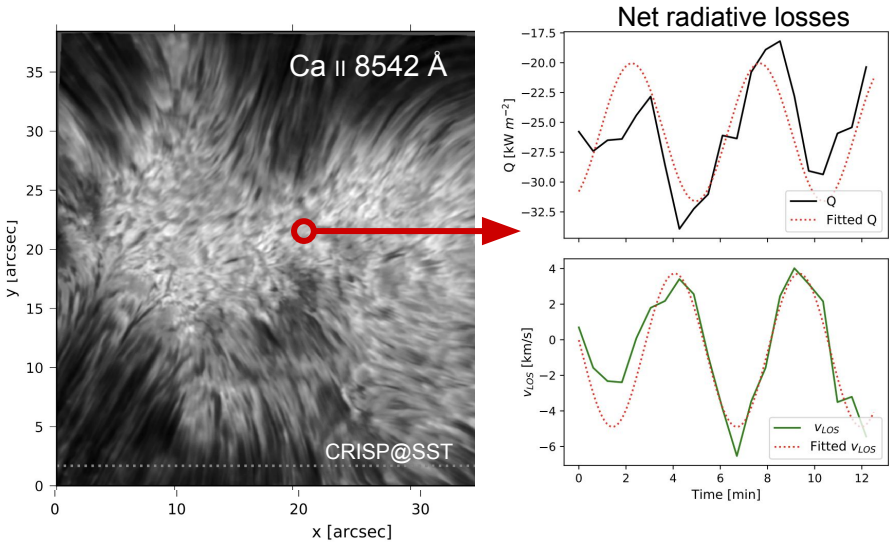
Accelerating the inference …

… in large FOVs



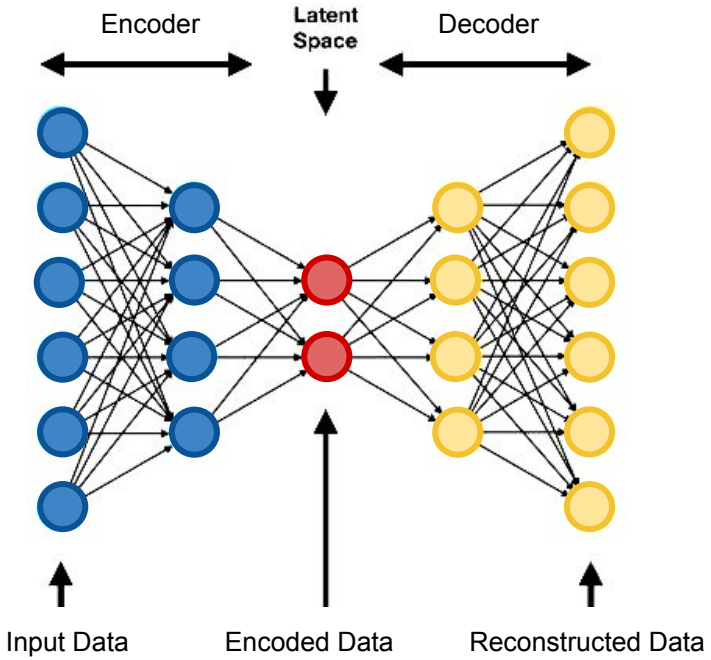
Kianfar S. et al. (2019)

… in long time-series

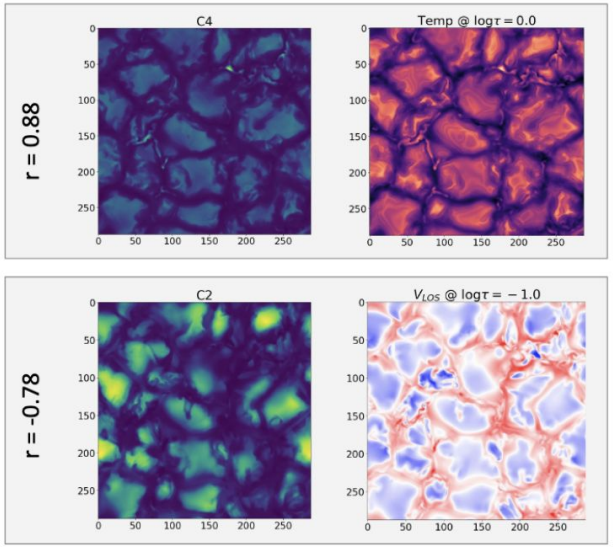


Morosin R. et al. (2022)

Autoencoders (the non-linear PCA)



Sparse Representation



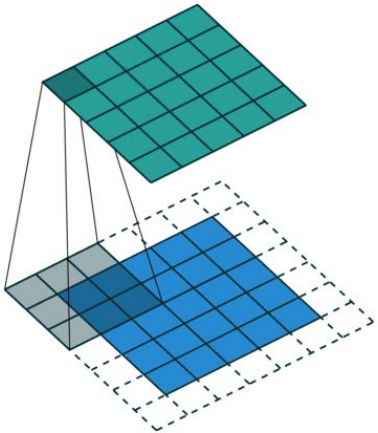
Flint S. & Milić I. (2021)

(e.g. Skumanich & López Ariste 2002; Sadykov et al. 2021; Sergey Ivanov et al. 2021)

If I want to analyze a megapixel image (10^6), do I need a neural network with O(>10^6) learnable parameters?

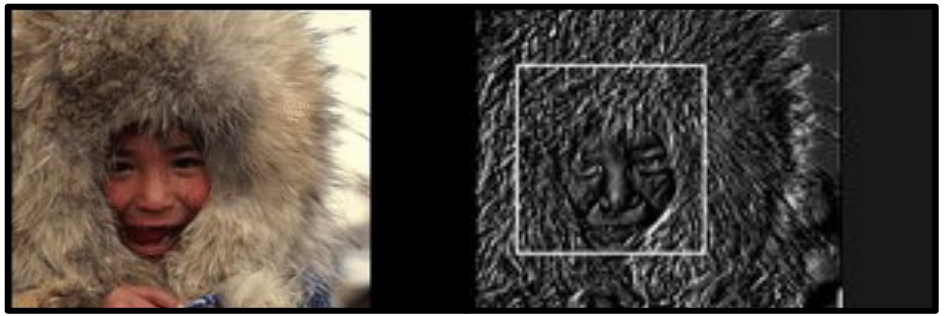
Convolutional Neural Networks

github.com/vdumoulin/



Input data

Output data



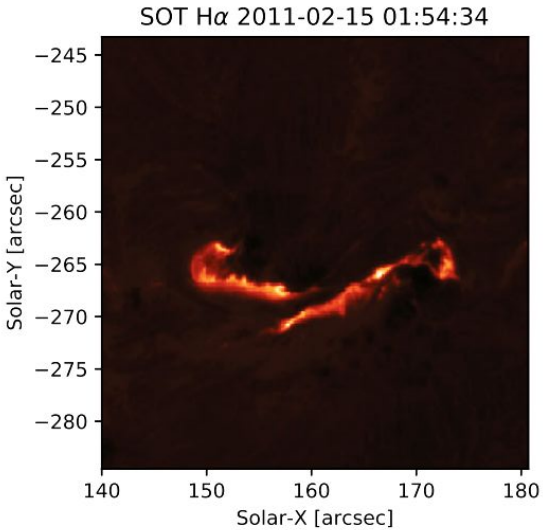
visual.cs.ucl.ac.uk/pubs/harmonicNets

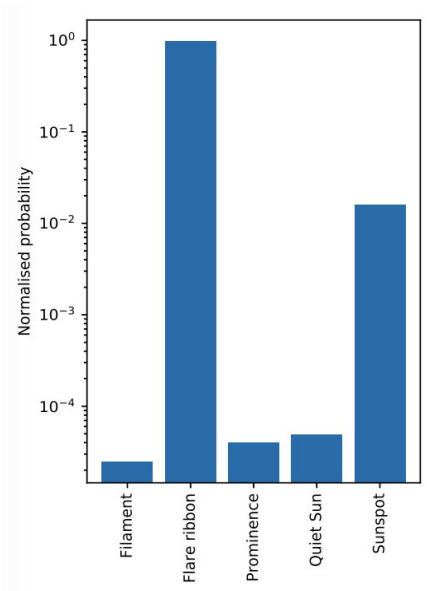
Translational Equivariance

$f(g(x))=g(f(x))$

The image as a “whole”

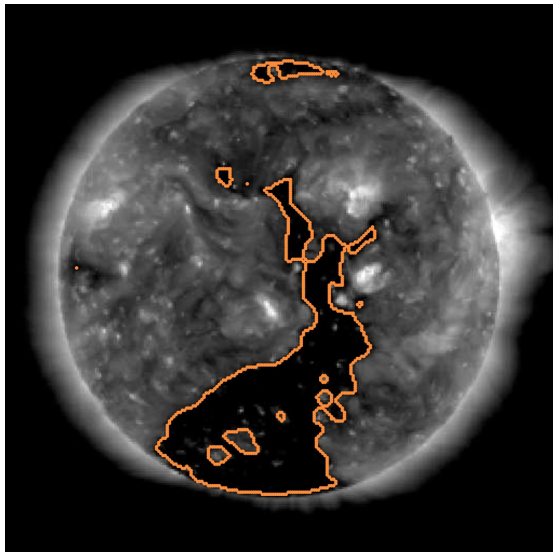
Automatic catalogues





Armstrong & Fletcher (2019)

Automatic segmentation

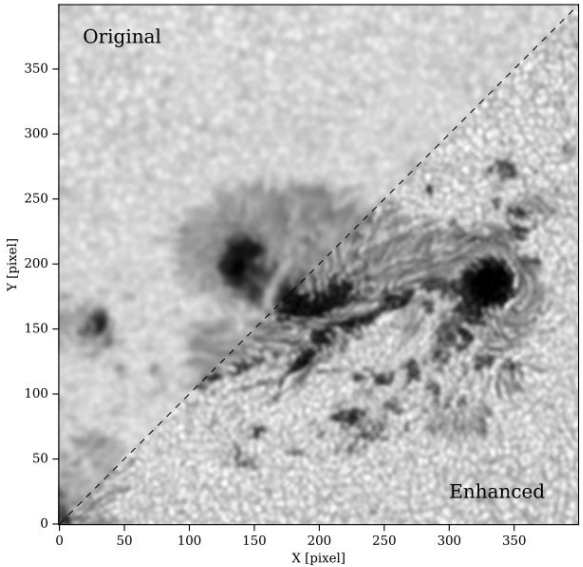


Illarionov & Tlatov (2018)

(e.g. Ahmadzadeh et al 2019; Zhu et al. 2019; Diercke et al 2022)

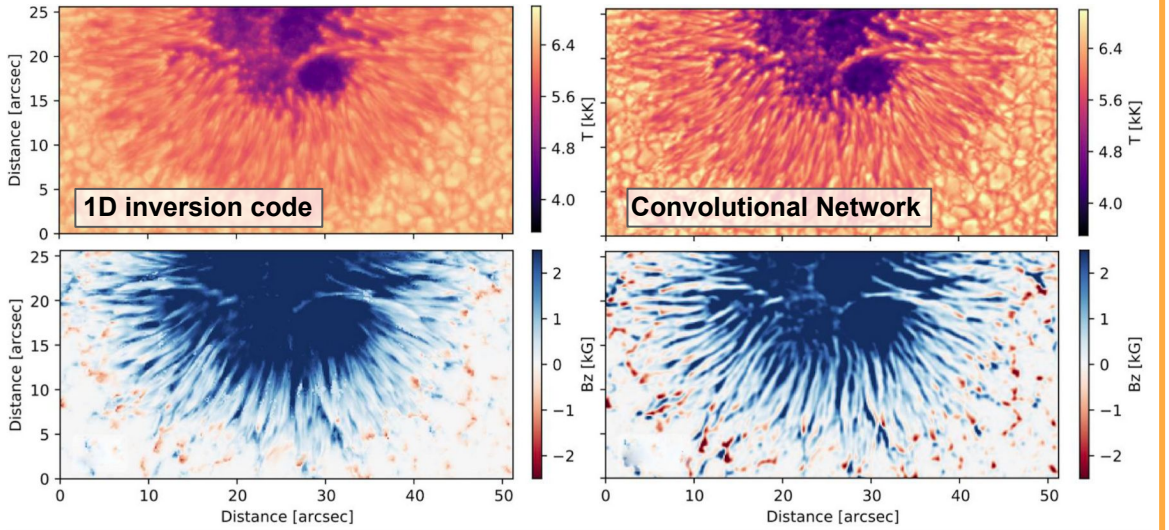
Using the information from nearby pixels

Image deconvolution



Díaz Baso et al. (2018)

Hinode PSF-compensated Stokes inversions

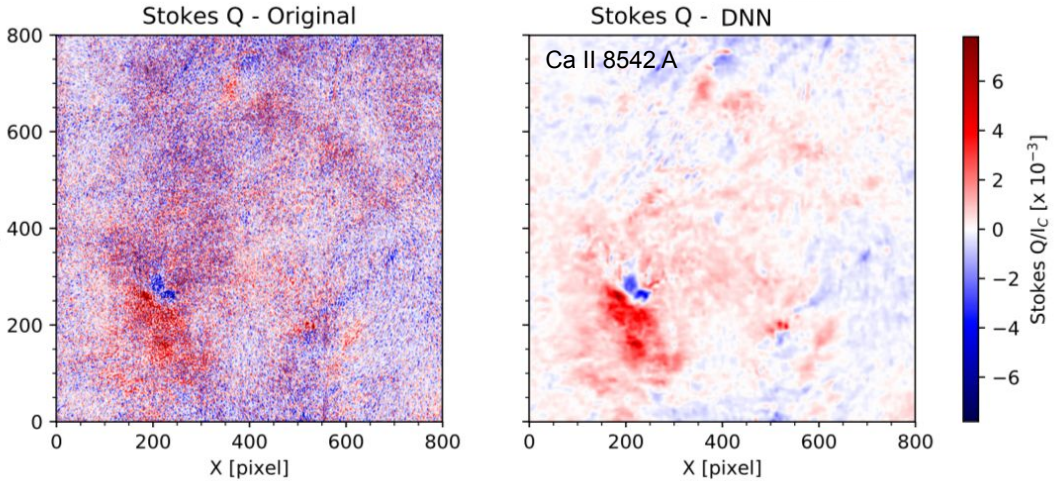


Asensio Ramos & Díaz Baso (2019)

(e.g. Asensio Ramos et al. 2018, 2021; Armstrong et al. 2021; Wang et al 2021; Deng et al 2021)

CNNs applications

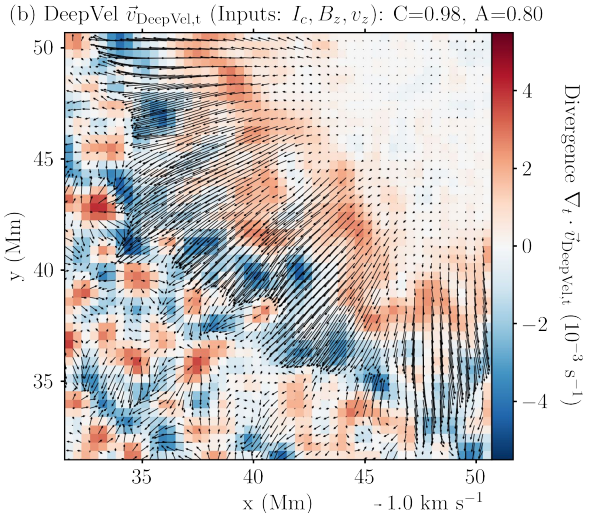
Solar image denoising



Díaz Baso et. al (2019)

(e.g. Eunsu Park et al. 2020)

Horizontal velocity fields

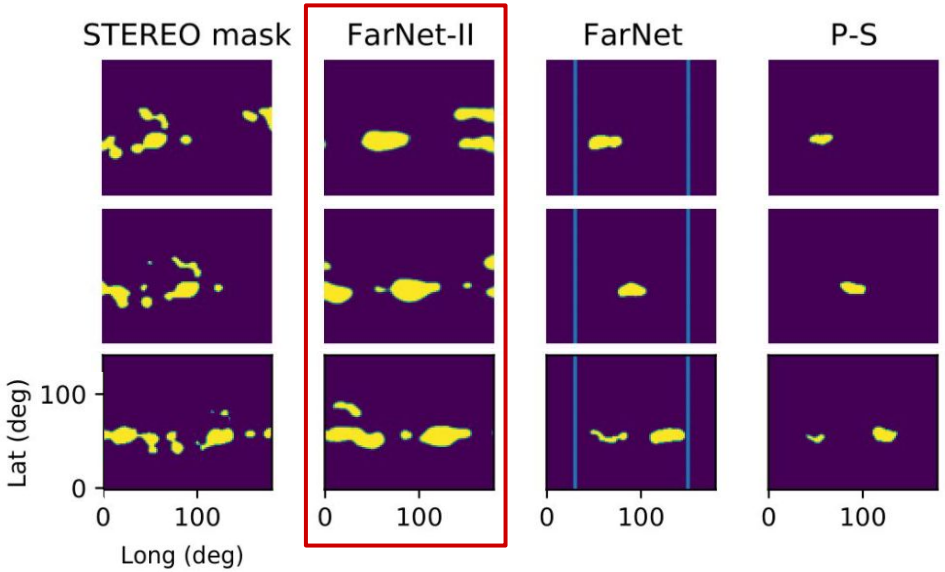


Benoit Tremblay et al. (2020, 2021)

(e.g. Asensio Ramos et al. 2017; Ishikawa et al., 2022)

Enhancing CNNs with temporal information

Far-side activity detection



Broock et al. (2022)

(e.g. Felipe et al. 2019; Broock et al 2021; Zeyu Sun et al. 2022)

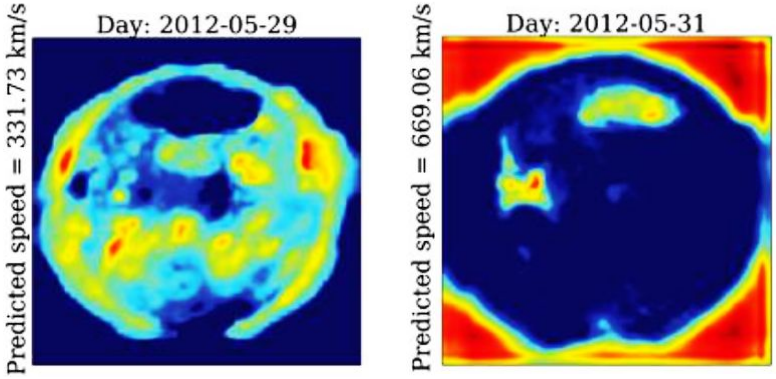
Challenges and future directions

- Why is this AR classified as a flare-producer?

<u>Interpretability</u>

To name a few methods:

- Learned Features
- Pixel Attribution (Saliency Maps)
- Testing Concepts
- Adversarial Examples
- Influential Instances
- Symbolic regression



Vishal Upendran et al. (2020)

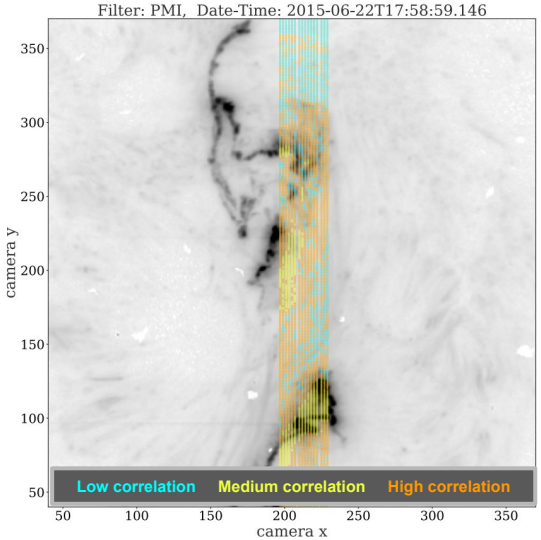
(e.g. Kangwoo Yi et al. 2021)

Does your method know when it doesn't know?

Uncertainty quantification

A probabilistic perspective: conditional information

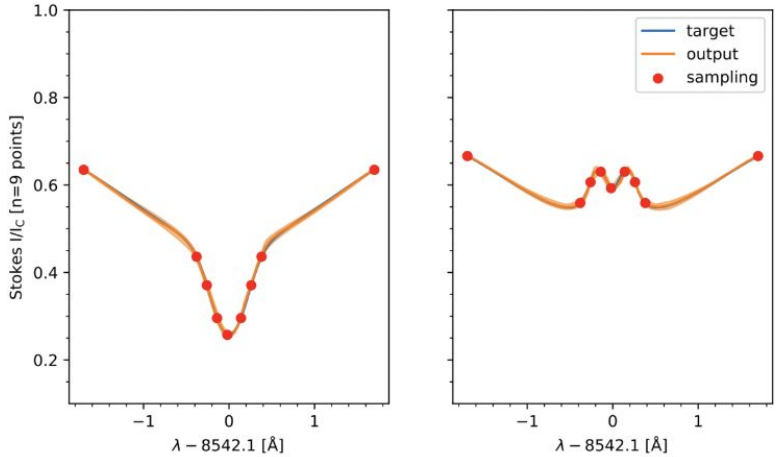
Mutual information



Panos et al. (2021a,b)

(e.g. Snelling et al. 2020)

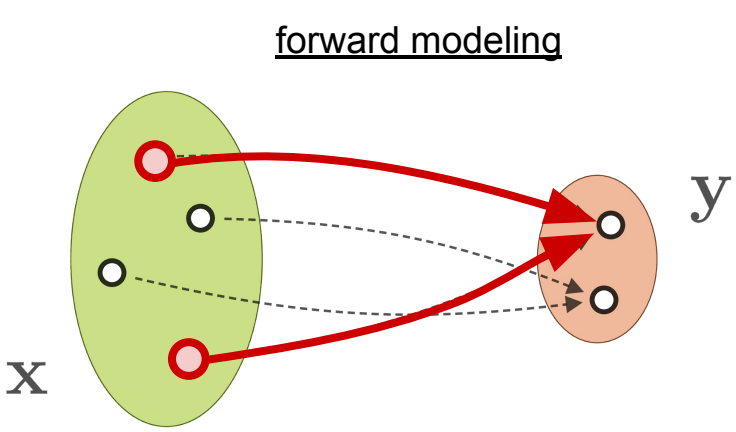
Designing observing sampling

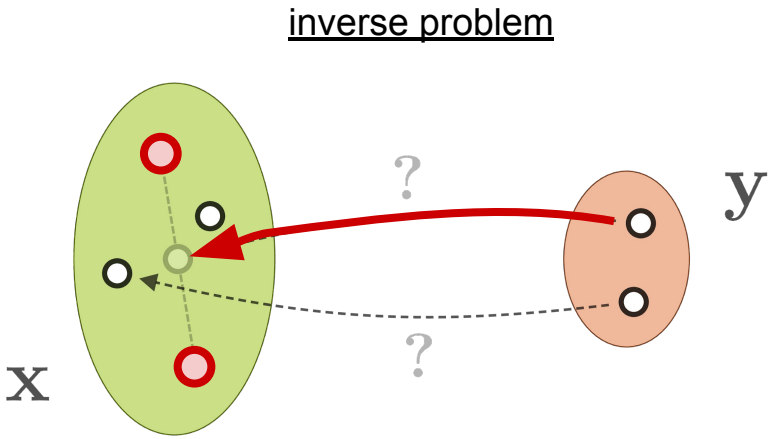


Díaz Baso et al. (in prep)

(e.g. Szenicer et al. 2019; Lim et al. 2021; Salvatelli et al. 2022)

A probabilistic perspective: inverse problems

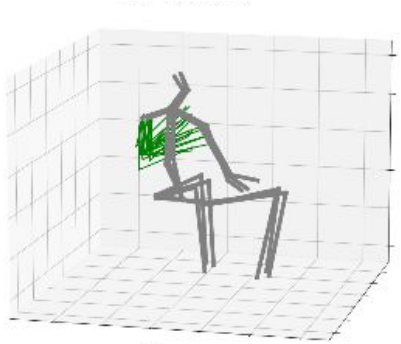




Inherent in many problems

Pose estimation

Input image



3D Pose

Wehrbein et al. (2021)

Super-Resolution

LR Input

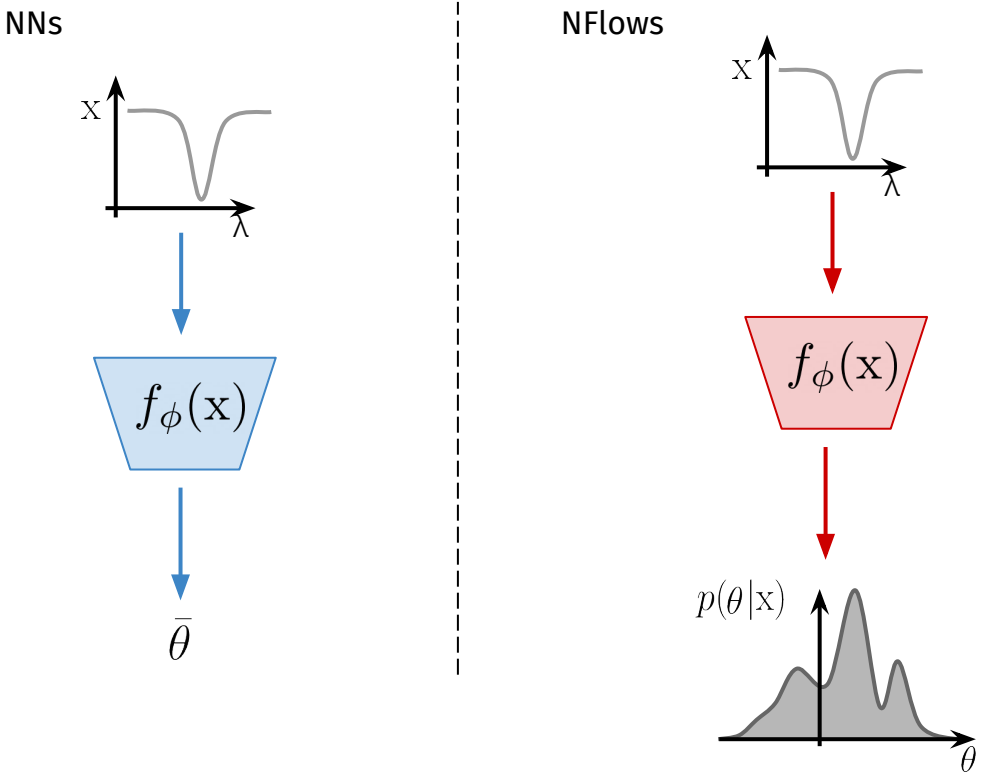
Input image

Output: Distribution

Lugmayr A. et al. (2020)

Normalizing flows

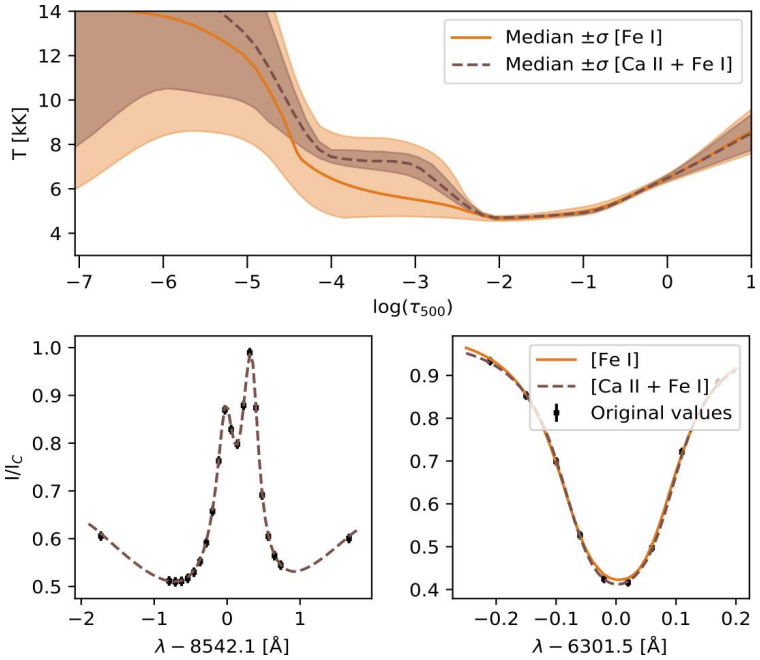
Rezende & Mohamed (2015), Dinh et al. (2016)



Normalizing flows

Rezende & Mohamed (2015), Dinh et al. (2016)

N-LTE inversion



Díaz Baso et al. (2021)

(e.g. Osborne et al. 2019, Asensio Ramos et al. 2021)

Normalizing flows → Diffusion models

Sohl-Dickstein et al. (2015), Yang & Ermon (2019), Ho et al. (2020)

Irish Terrier riding a horse in Patagonia and playing the harmonica

Cat with a yellow hat going down the stairs under water

Panda mad scientist mixing sparking chemicals, artstation

Grizzly bear taking a selfie on the Golden Gate bridge on a windy day

Ramesh et al. (2022)

→ valuable effort in complex inverse problems.

Summary and conclusions

- Machine learning can help in many different ways: **explore patterns, image reconstruction, compression, denoising, parameter inference, classification, and tracking,** etc. Inference is extremely fast.

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- Machine learning can help in many different ways: **explore patterns, image reconstruction, compression, denoising, parameter inference, classification, and tracking,** etc. Inference is extremely fast.

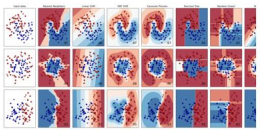
- The question you want to address is as important as the method. Depending on the goal, no need to always "reinvent the wheel" (**literature vs own design**).

(e.g. scikit-learn - python)

Classification

Identifying which category an object belongs to.

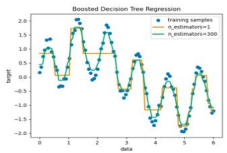
Applications: Spam detection, image recognition.
Algorithms: SVM, nearest neighbors, random forest, and more...



Regression

Predicting a continuous-valued attribute associated with an object.

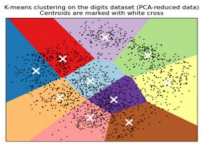
Applications: Drug response, Stock prices.
Algorithms: SVR, nearest neighbors, random forest, and more...



Clustering

Automatic grouping of similar objects into sets.

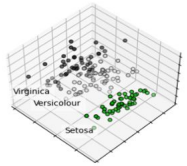
Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, and more...



Dimensionality reduction

Reducing the number of random variables to consider.

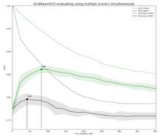
Applications: Visualization, Increased efficiency
Algorithms: PCA, feature selection, non-negative matrix factorization, and more...



Model selection

Comparing, validating and choosing parameters and models.

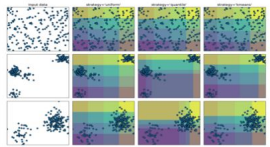
Applications: Improved accuracy via parameter tuning
Algorithms: grid search, cross validation, metrics, and more...



Preprocessing

Feature extraction and normalization.

Applications: Transforming input data such as text for use with machine learning algorithms.
Algorithms: preprocessing, feature extraction, and more...



Summary and conclusions

- Machine learning can help in many different ways: **explore patterns, image reconstruction, compression, denoising, parameter inference, classification, and tracking,** etc. Inference is extremely fast.

- The question you want to address is as important as the method. Depending on the goal, no need to always "reinvent the wheel" (**literature vs own design**).

- There are still many ways to improve them: incorporating **physical constraints** (e.g. symmetries, conservation laws), making them **interpretable**, quantifying **uncertainty**, enabling **multimodal** solutions, etc.

What a time to be alive!

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