Building a Robot Judge:
Data Science for Decision-Making

12. Encoders and Explanations

Q&A Page

https://bitly.com/BRJ_Padlet12

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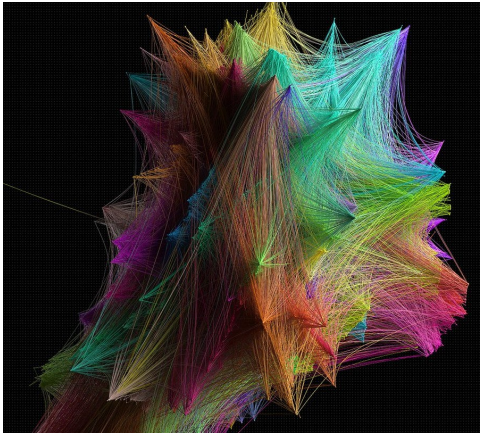
2. explaining the predictions of classifiers and regressors

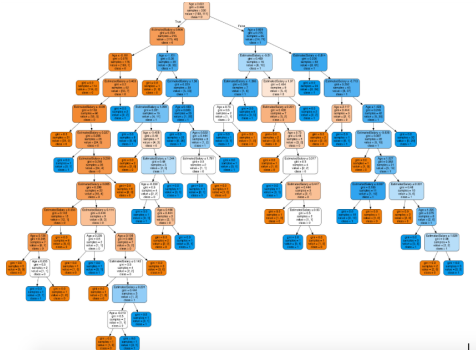
We will see that these are highly overlapping tasks. Interpretability/explainability is a major benefit of dimensionality reduction.

High-dimensional datasets and machine learning models are black boxes

High-Dimensional Datasets

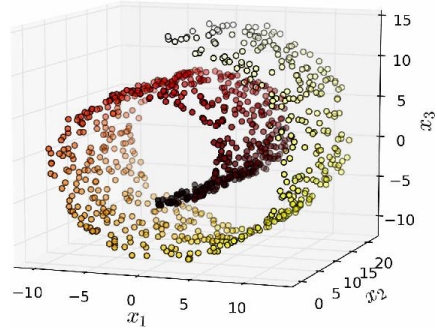


Big ML Models



"The Swiss Roll"

- Datasets are not distributed uniformly across the feature space.
- They have a lower-dimensional latent structure – a **manifold** – that can be learned.



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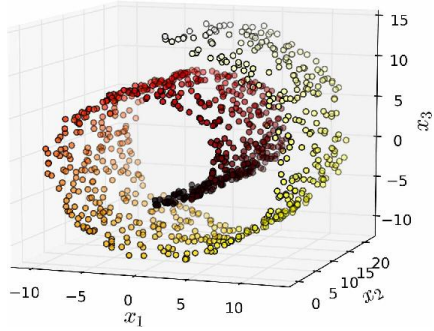

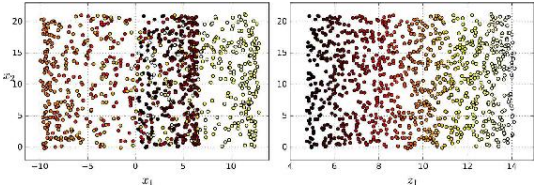

- **Dimensonality reduction** makes data more interpretable – for example by projecting down to two dimensions for visualization.
- improves computational tractability.
- can improve model performance.

Explaining Model Predictions

(a) Husky classified as wolf

(b) Explanation

Figure 11: Raw data and explanation of a bad model's prediction in the "Husky vs Wolf" task.

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← for example, classifying a dog image as a wolf because there is snow in the background (a correlated feature).

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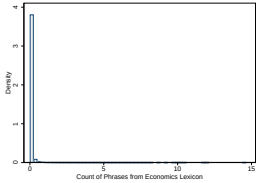
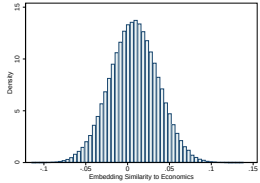
- These problems, along with the black box nature of ML models, is a major hurdle to making these technologies trustworthy enough to use to support high-stakes decisions, like those in courts.

A lot of what we do is interpreting/explaining

Summary statistics / plotting data:





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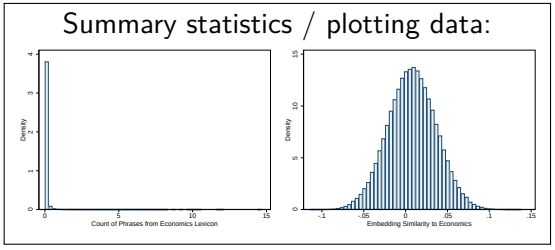

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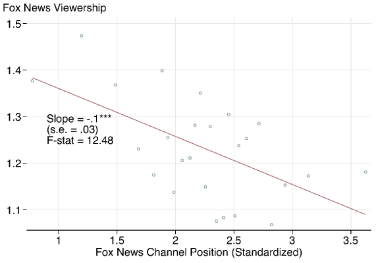

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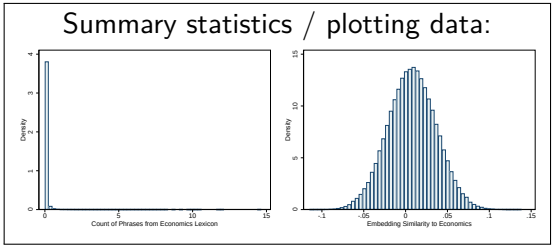

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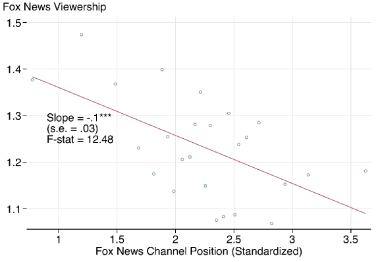

Event study plots "explain"
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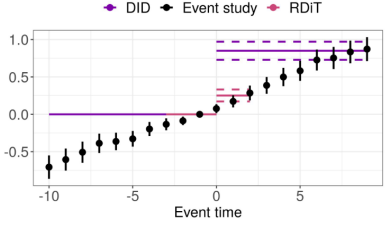

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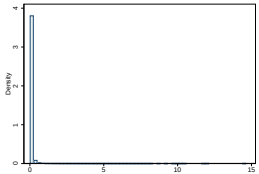

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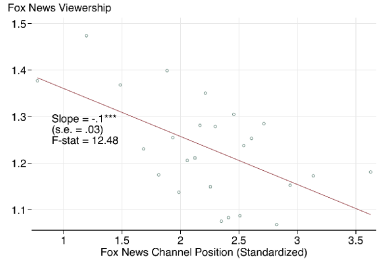

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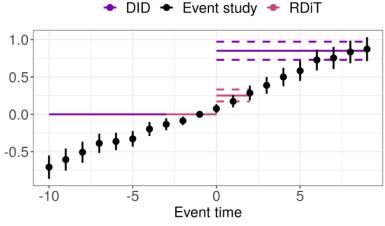
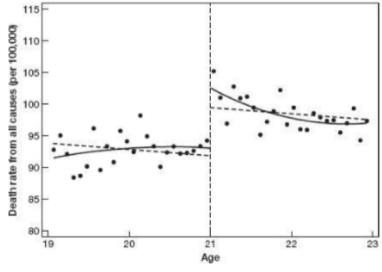


Regression discontinuity plots "explain" regression discontinuity estimates:



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- **Selective**: explanations should be short
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  - e.g., different explanation for data scientists vs for lawyers.
- **Contrastive**: explains not just why a certain prediction was made, but why it was made instead of other predictions.

Linear Models

- Linear models (e.g. linear regression, logistic regression) are (relatively) interpretable:
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  - excludes interactions $\rightarrow$ often have bad ML performance

Feature Importance / Selection

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Feature selection can be done as a pre-processing step:

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from sklearn.feature_selection import SelectKBest, chi2
selector = SelectKBest(chi2, k=10)
X_train_filtered = selector.fit_transform(X_train,y_train)
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- `chi2, f_classif, and f_regression` measure linear correlations. Mutual information captures higher-order dependencies (**`mutual_info_classif`**, **`mutual_info_regression`**). Slower to compute.

Visualizing Marginal Effects on Predictions: Partial Dependence Plots

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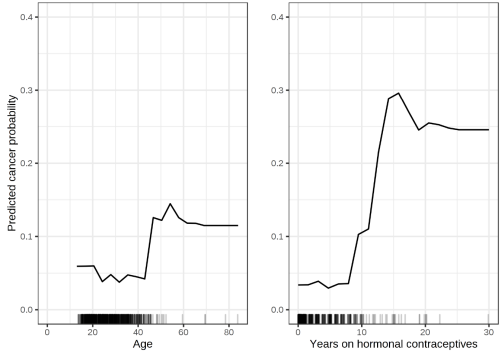

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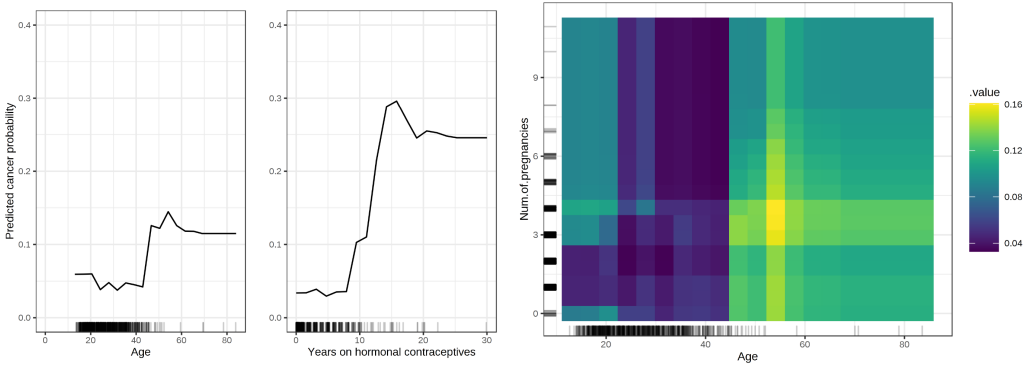

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Solution: **Permutation feature importance** (Fisher, Rudin, and Dominici 2018):

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Apply to trained `model` using test set:

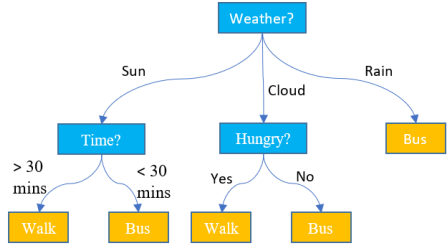
```
from eli5.sklearn import PermutationImportance
perm = PermutationImportance(model)
perm.fit(X_test, y_test)
eli5.show_weights(perm)
```

Out[20]:

Weight	Feature
0.4700 ± 0.0614	OverallQual
0.1439 ± 0.0156	GrLivArea
0.0499 ± 0.0034	2ndFlrSF
0.0363 ± 0.0091	TotalBsmtSF
0.0294 ± 0.0032	1stFlrSF
0.0271 ± 0.0102	BsmtFinSF1
0.0166 ± 0.0028	Fireplaces
0.0130 ± 0.0068	GarageArea
0.0130 ± 0.0044	YearBuilt
0.0115 ± 0.0071	LotArea
0.0105 ± 0.0048	GarageCars
0.0105 ± 0.0048	YearRemodAdd

Trees and Tree Ensembles

- Small decision trees have the advantage of being highly interpretable.



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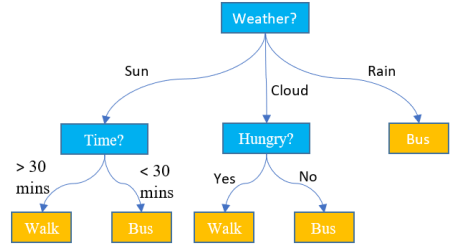

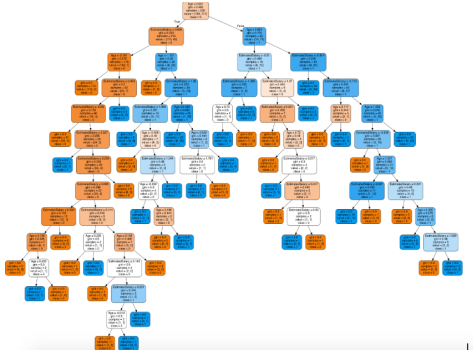

- Larger trees and ensembles (e.g. XGBoost) lose this nice feature.
- Best-performing ML models are hard to interpret because they use lots of features and exploit non-linearities and interactions.

Interpreting Tree Ensembles

XGBoost's Feature Importance Metric:

- At each decision node, compute **information gain** for feature j **(change in predicted probability**).
- Average across all nodes for each j.

Ranks predictors by their relative contributions.

```
from xgboost import plot_importance
plot_importance(xgb_reg, max_num_features=10)
```

Example: Most Important Budget Features for Corruption Prediction

(Ash, Galletta, Giommoni 2020)

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Category	Macro Category	Weight	Category	Macro Category	Weight
Assets	Assets	330	Outstanding loan credit	Assets	69.4
Financial assets	Assets	182	Tax on industrialized products	Revenue	69
Population		142.6	**Property tax on land/buildings**	Revenue	68
Cash	Assets	116.4	Liquid assets	Assets	67.8
Spending in agriculture	Expenditure	94.8	Civil servant per diems	Expenditure	67.4
Property tax on rural land	Revenue	89.6	Spending for legislative procedure	Expenditure	65
Bank deposit	Assets	85.4	Taxes	Revenue	64.4
Motor vehicle property tax (from FG)	Revenue	72.8	Budget deficit		63
Transf. of ownership tax	Revenue	72	Non financial current asset	Assets	60.6
Spending in transportation	Expenditure	72	**Capital expenditure**	Expenditure	60

Important Features tend to show up in Audit Reports

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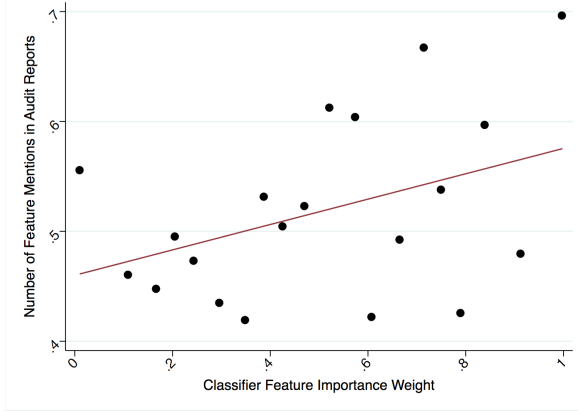

Notes: Binscatter for frequency that budget feature appears in the municipal audit reports (vertical axis) against binned feature importance weights for each feature (horizontal axis). Pearson's correlation is 0.17 (.24 for the log measures, rather than ranks). Slope coefficient is 0.112 with p=.03 (robust standard errors).

Activity 12.1: Poll / Padlet Applying Feature Importance

PCA (principal component analysis) / SVD (singular value decomposition)

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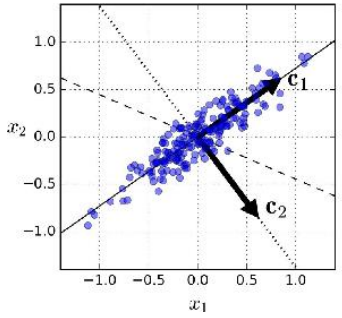

- PCA computes the dimension in data explaining most variance.

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from sklearn.decomposition import PCA
pca = PCA(n_components=10)
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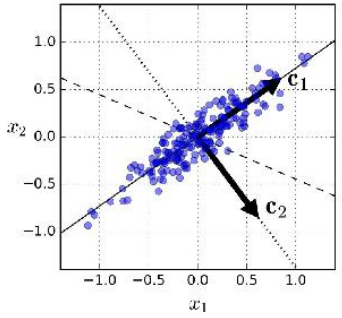

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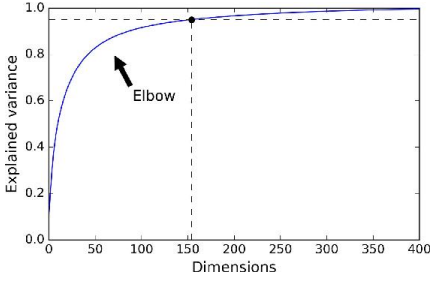

- after the first component, subsequent components learn the (orthogonal) dimensions explaining most variance in dataset after projecting out first component.

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- PCA might destroy (a lot of) predictive information in your dataset.
  - compromise: use feature selection to keep strong predictors, and take principal components of weak predictors.
- dimensions are not interpretable.
  - For non-negative data (e.g. counts or frequencies), **Non-negative Matrix Factorization (NMF)** provides more interpretable factors than PCA.

Dimension Reduction for Visualization: t-SNE and MDS

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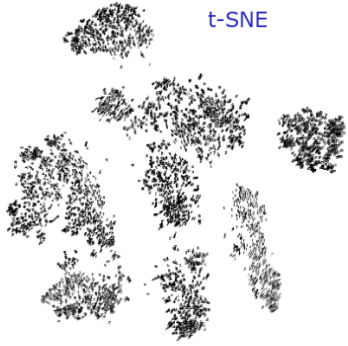

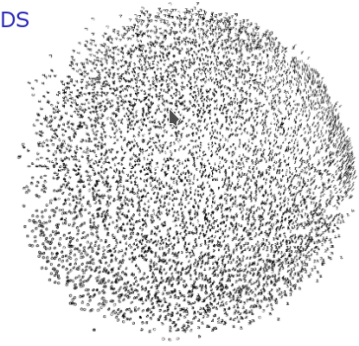

From: L. Van der Maaten & G. Hinton, Visualizing Data using t-SNE, Journal of Machine Learning Research 9 (2008) 2579-2605

- **t-Distributed Stochastic Neighbor Embedding (t-SNE)** tries to keep similar observations close and dissimilar observations apart.
  - Useful for visualizing clusters of observations in high-dimensional space
- **Multidimensional Scaling (MDS)** tries to preserve distances between observations .

k-means clustering separates observations into k groups

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- Matrix of predictors treated as a Euclidean space (should standardize all columns)
- algorithm: initialize cluster centroids randomly, then shift around to minimize sum of within-cluster squared distance

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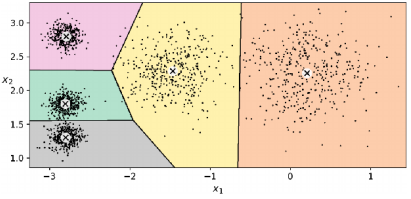

K-Means decision boundaries (Voronoi tessellation)

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from sklearn.cluster import Kmeans
kmeans = KMeans(n_clusters=10)
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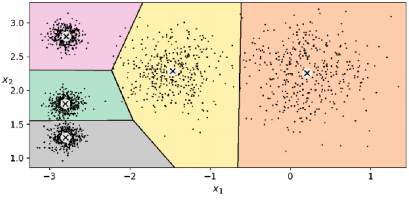

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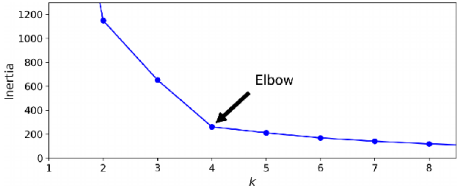
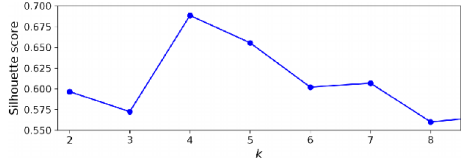
k (number of clusters) is the only hyperparameter, can select using:



Selecting the number of clusters k using the "elbow rule"



Selecting the number of clusters k using the silhouette score

Other clustering algorithms

- "k-medoid" clustering use L1 distance rather than Euclidean distance; produces the "medoid" (median vector) for each cluster rather than "centroid" (mean vector).
  - less sensitive to outliers, and medoid can be used as representative data point.

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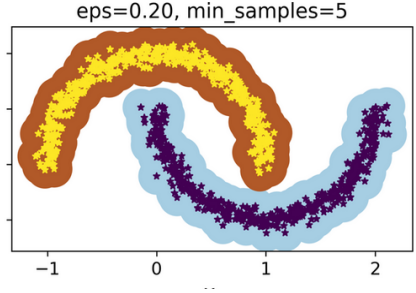
  - detects and excludes outliers automatically



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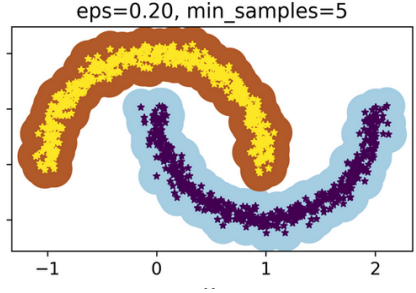


- Agglomerative (hierarchical) clustering makes nested clusters.

Clusters Provide Prototypes

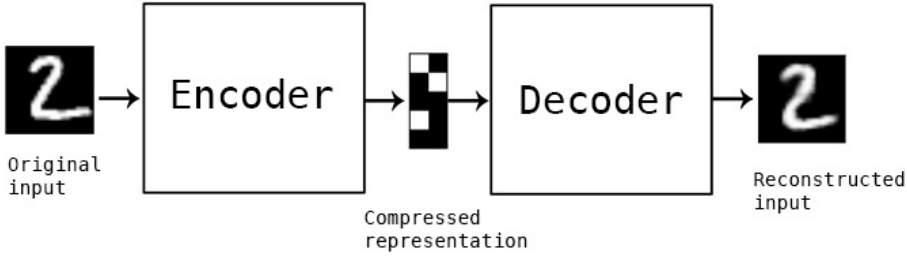
- Clustering can be used for description / explanation:
  - show selected variable values from centroid (even better, medoid) data points
  - medoids for large clusters are representative "prototypes" for the whole dataset (Molnar ch. 6.3).

Clusters Provide Prototypes

- Clustering can be used for description / explanation:
  - show selected variable values from centroid (even better, medoid) data points
  - medoids for large clusters are representative "prototypes" for the whole dataset (Molnar ch. 6.3).
- Conversely, data points that don't fit well into a cluster (far from any centroid, or dropped by dbscan) are outliers ("criticisms").

Autoencoders: Optimal Compression Algorithms

- Autoencoders = neural nets that perform optimal domain-specific lossy compression:



- Learned encodings can be decoded back to a *reconstruction* – a (minimally) lossy representation of the original data.

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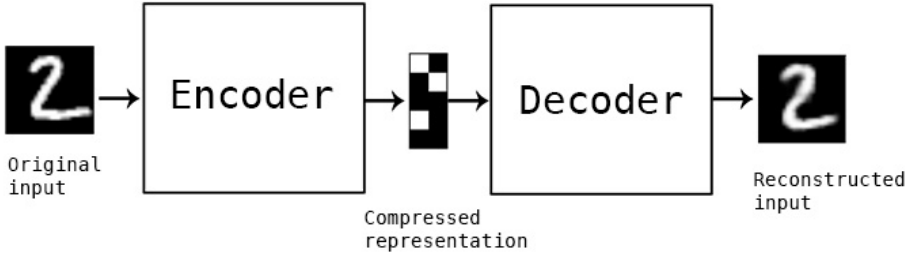


- Learned encodings can be decoded back to a *reconstruction* – a (minimally) lossy representation of the original data.
- AE's can memorize complex, unstructured data.

Autoencoder Architecture

- Stacked layers gradually decrease in dimensionality to create the compressed representation
- then gradually increase in dimensionality to try to reconstruct the input.
- can “tie weights” to make encoding layers and decoding layers symmetric.

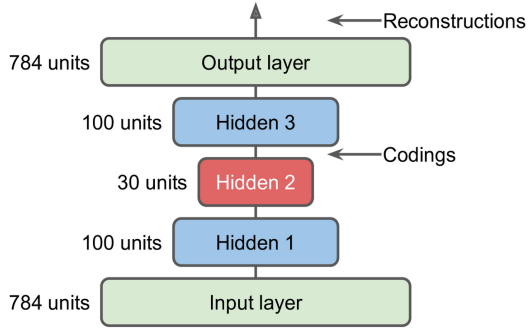


Figure 17-3. Stacked autoencoder

Reconstruction from encoded vector

Figure 17-4. Original images (top) and their reconstructions (bottom)

Autoencoders for Data Visualization

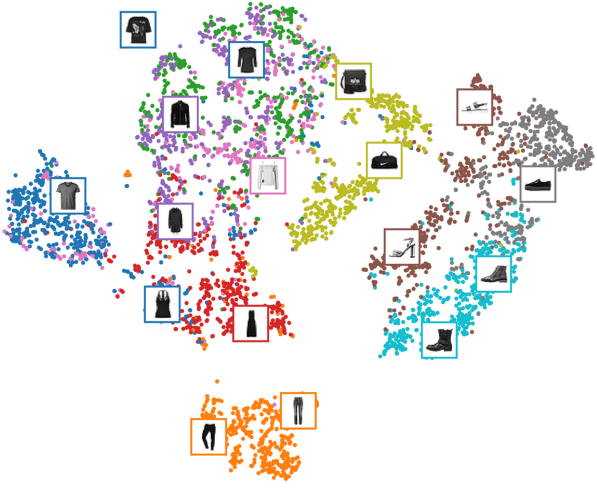
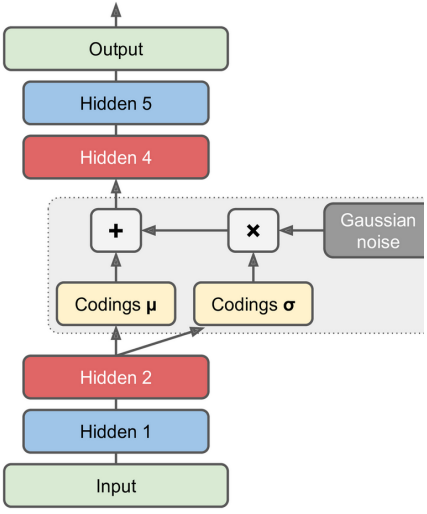


Figure 17-5. Fashion MNIST visualization using an autoencoder followed by t-SNE

- Decent baseline for visualizing the encodings:
  - use an autoencoder to compress your data to relatively low dimension (e.g. 32 dimensions)
  - then use t-SNE for mapping the compressed data to a 2D plane.

Variational Autoencoders

Encodings taken as parameters of a gaussian (means μ and variances σ^2)



Decoder draws from the distribution to produce first layer.

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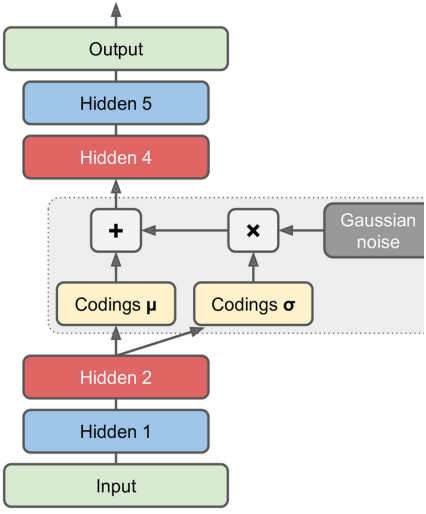

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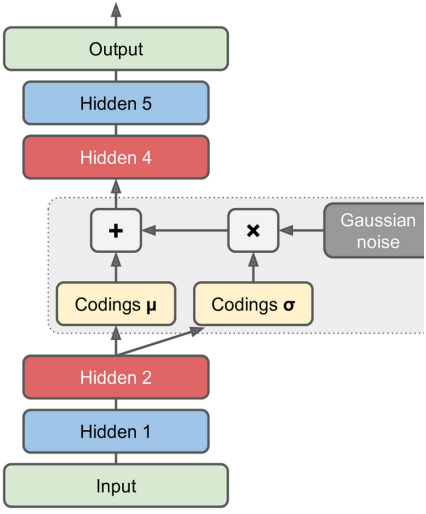
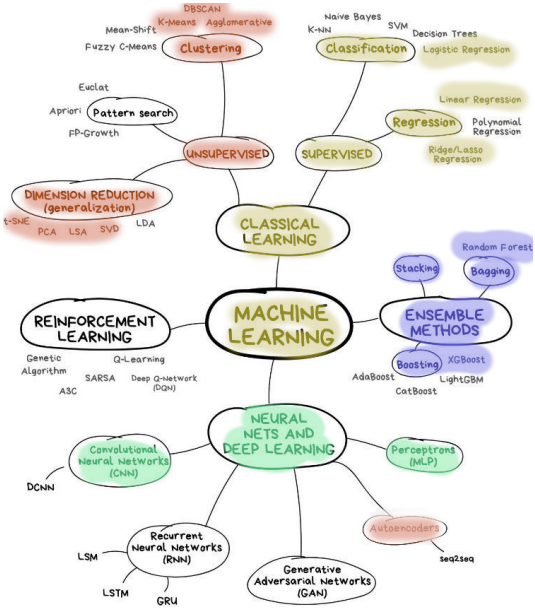


Decoder draws from the distribution to produce first layer.

- Can then sample from the normal distribution (or just choose numbers) and generate reconstructions.
- VAE's do *semantic interpolation*: picking an encoding vector between two encodings will produce a reconstruction that is "between" the associated images

Recap: The ML Landscape



Activity 2.2: Sentence Placement

I picked a sequence of five sentences from a paper on ML interpretability. Put sentences 2-5 in the correct order:

1. Machine learning systems are becoming increasingly ubiquitous.
2. However, most of these accurate decision support systems remain complex black boxes, meaning their internal logic and inner workings are hidden to the user and even experts cannot fully understand the rationale behind their predictions.
3. The research community has recognized this interpretability problem and focused on developing both interpretable models and explanation methods over the past few years.
4. Moreover, new regulations and highly regulated domains have made the audit and verifiability of decisions mandatory, increasing the demand for the ability to question, understand, and trust machine learning systems, for which interpretability is indispensable.
5. These systems's adoption has been expanding, accelerating the shift towards a more algorithmic society, meaning that algorithmically informed decisions have greater potential for significant social impact.

Global Surrogate Model Explanation

Approximate a black box model with an interpretable model

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Global Surrogate Model Explanation

Approximate a black box model with an interpretable model

1. Get predictions $\hat{y}$ of the black box model from the data X.
2. Train an interpretable model (lasso, decision tree, etc) on X with $\hat{y}$ as the label.
3. Validate that the surrogate model replicates the predictions of the black box model
   - e.g., compute R^2 between black box $\hat{y}$ and surrogate $\hat{\hat{y}}$

Local Feature Importance

Local Surrogate Model
(LIME = local interpretable model-agnostic explanations.)

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Shapley Values

Assigns importance to features by relative contribution to prediction (complicated formula based on solution concept in game theory)

- (sometimes) better than LIME because accounts for interactions
- slower to compute
- default local importance metric on Google AI Platform

Interpreting Image Classifiers: Gradient Heat Maps

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Example from "DeepConnection" paper predicting whether couples in images are happy or unhappy:

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- that is, for ML prediction function $\hat{y}(\cdot)$, find counterfactual X' that solves

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where $d(\cdot)$ is a distance metric and $\lambda \geq 0$ calibrates the relative importance of label change and feature distance.

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  2. Standardize all features by their respective *mean absolute deviation*, so dimensions are comparable in L1 space.
- The mlxtend package makes this easy to do:

```
from mlxtend.evaluate import create_counterfactual
x_prime = create_counterfactual(x_reference=x_ref, # current data point
                                y_desired=1, # alternative outcome
                                model=clf, # trained model
                                X_dataset=X, # dataset
                                lammbda=1) # hyperparameter
```

Extensions

- Dandl et al (2020) improve on the Wachter et al objective in three ways:
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  1. use Gower distance, rather than L1 distance, to allow for categorical features.
  2. penalize the number of predictors that are changed, to encourage changes along relatively few dimensions.
  3. reward counterfactuals that are likely to be possible – measured by how close they are to at least one observed data point.

Activity 12.3: Breakout Groups: Explanations for Decision Support

https://bit.ly/2JRbQgx