UCLA QCBio Collaboratory

Machine Learning with Python

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2023 Spring

UCLA Bioinformatics

Thanks Dr. Seyoon Ko for some code materials

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Day 3: Unsupervised learning

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Agenda

- Day 1: Introduction to machine learning
  - Some key concepts in machine learning
  - Jupyter notebook and some packages usage
- Day 2: Supervised learning
  - Classification
  - Regression
  - Regularization
- Day 3: Unsupervised learning
  - Dimension reduction
  - Clustering

Notation of the slides

- `Code or Pseudo-Code chunk` starts with "➢", e.g.
  - ➢ `print("Hello world!")`

- Link is underlined

- Important terminology is in **bold** font

Overview

Time

- 3-hour workshop (45min + 45min + 30min + practice/Q&A)

Topics

- ❑ Regression
- ❑ Regularization
- ❑ Dimension reduction
- ❑ Clustering

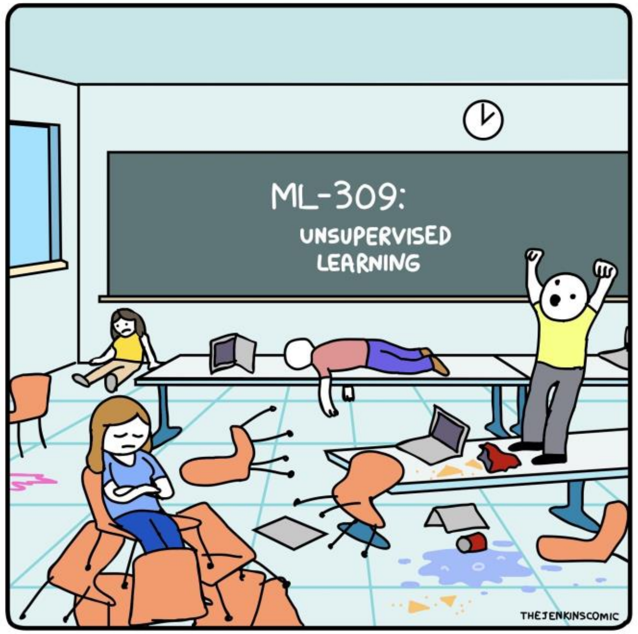


Image from internet

Summary –Day2

Classification:

- ❑ 9 different classification algorithms
    - Logistic regression
    - KNN
    - Naïve bayes
    - Support vector machine
    - Decision tree
    - Random forest
    - Adaboost
    - Gradient boosting
    - Neural network

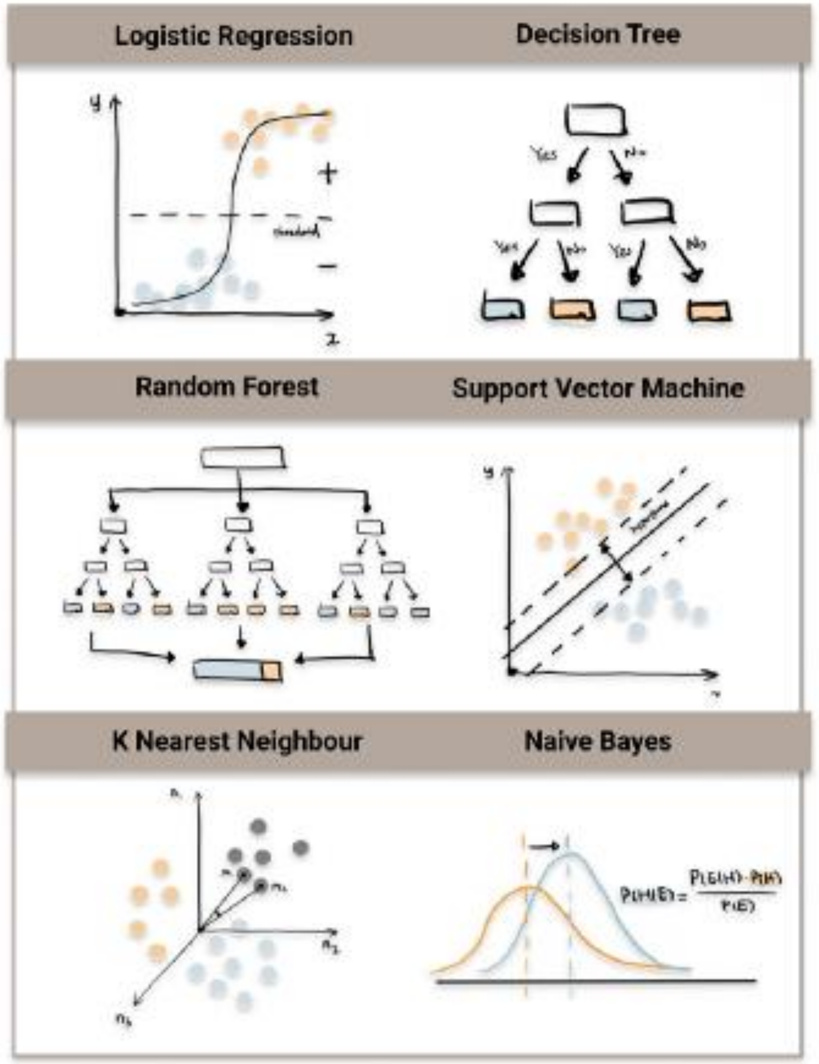


Image from internet

Summary –Day2

Classification:

- ❑ 9 different classification algorithms
- ❑ Cross entropy loss function

True probability distribution
(one-hot)

$$H(p,q) = -\sum_{x\in\text{classes}} p(x)\log q(x)$$

Your model's predicted
probability distribution

Summary –Day2

Classification:

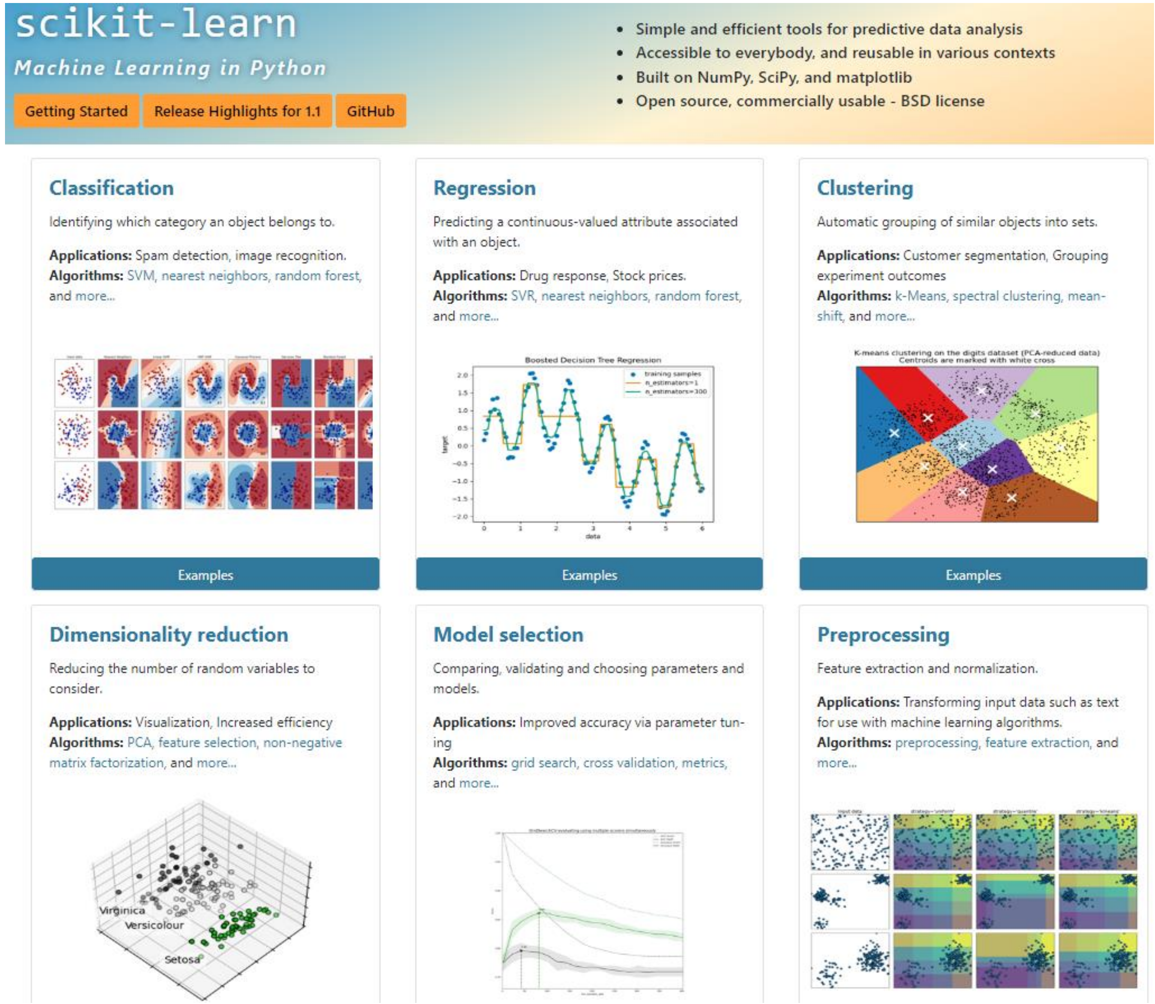
- ❑ 9 different classification algorithms
- ❑ Cross entropy loss function
- ❑ Performance measure
  - Accuracy
  - Confusion matrix
  - Precision & Recall
  - ROC, AUC, PR-ROC

		Predicted Class		
		Positive	**Negative**	
Actual Class	**Positive**	True Positive (TP)	False Negative (FN) **Type II Error**	**Sensitivity** $\frac{TP}{(TP+FN)}$
	Negative	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
		Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

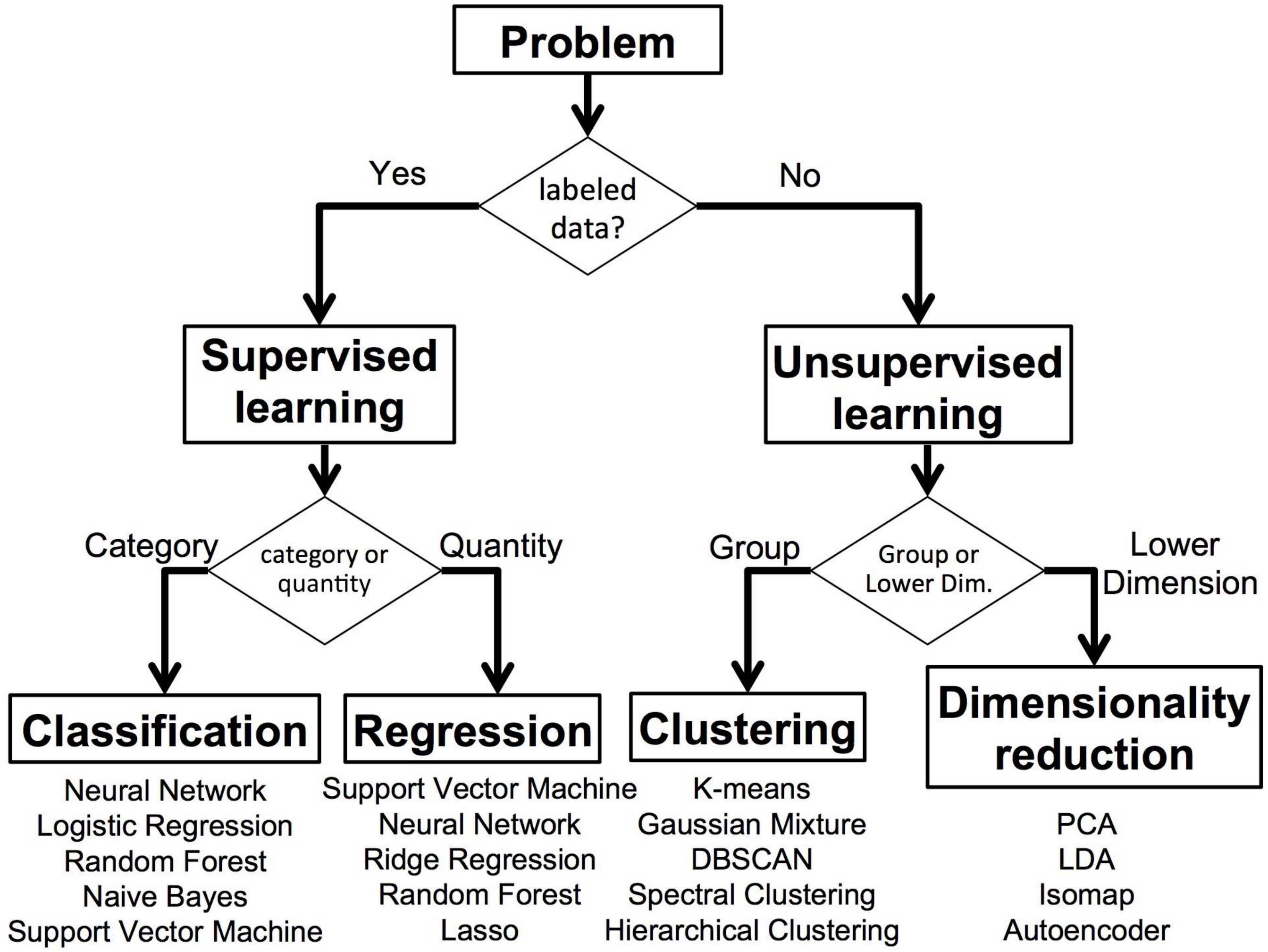
Summary –Day2

Classification:

- ❑ 9 different classification algorithms
- ❑ Cross entropy loss function
- ❑ Performance measure
- ❑ Practice
  - Training-test-validation set construction
  - Performance measure calculation
  - ROC curve, decision boundary
  - Linearly non-separable example
  - Parameter tuning (overfitting/underfitting)



Types of machine learning



https://pythonnumericalmethods.berkeley.edu/notebooks/chapter25.01-Concept-of-Machine-Learning.html

Supervised learning

- Training data with n ***samples*** of ***features*** **x** and ***labels*** y
- Learn a function class f(**x**) to describe y based on **x**

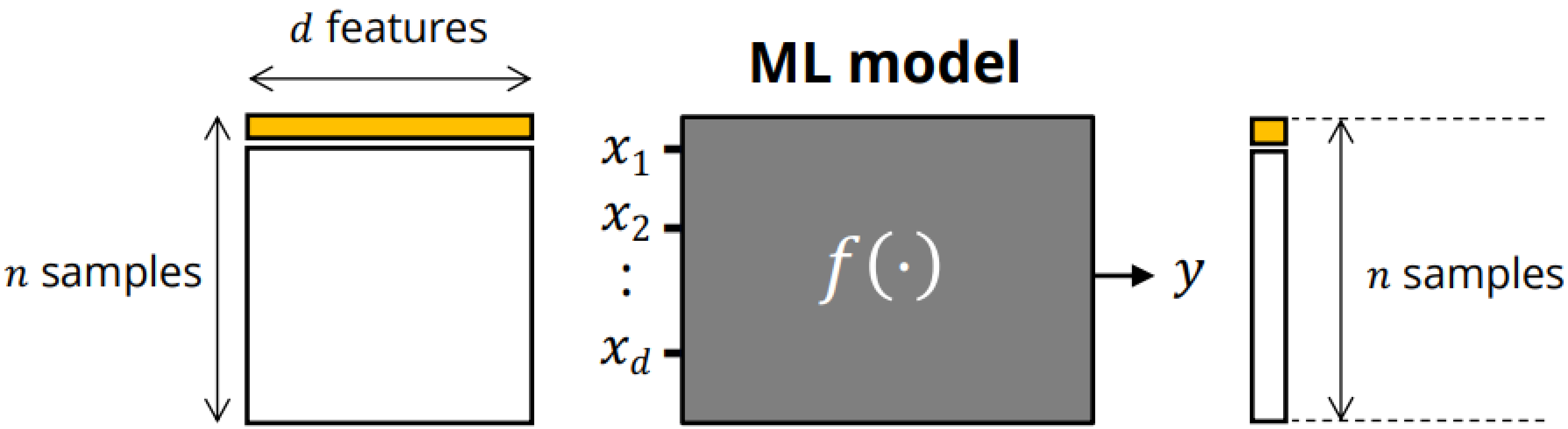
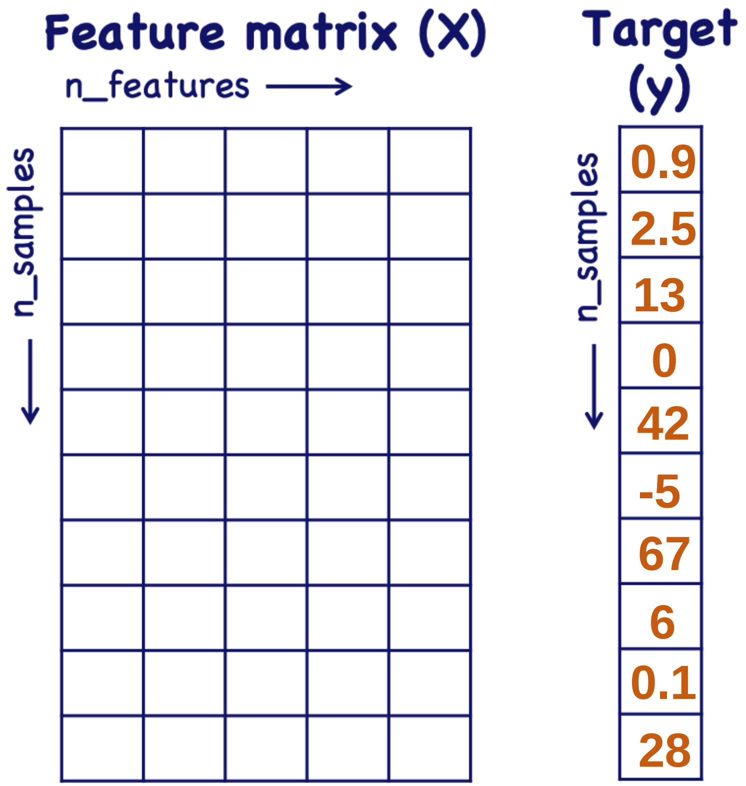


Figure adopted from CSEP 590B Explainable AI

Different choice of f() for regression tasks

- Linear regression
- Polynomial regression
- SVR
- Tree-based regression
- Boosting
- Neural Network

  …



$$\hat{y} = f(x)$$

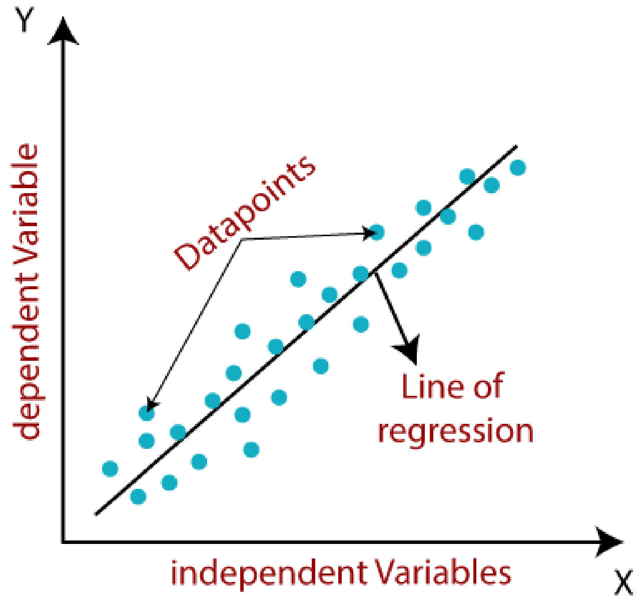
https://pythonnumericalmethods.berkeley.edu/notebooks/chapter25.01-Concept-of-Machine-Learning.html

Linear regression

- Make prediction by computing the weighted sum of features

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

$$\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x}$$



Linear regression

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$$\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x}$$

- Train the model: find a parameter set to best fit the data

- Loss function

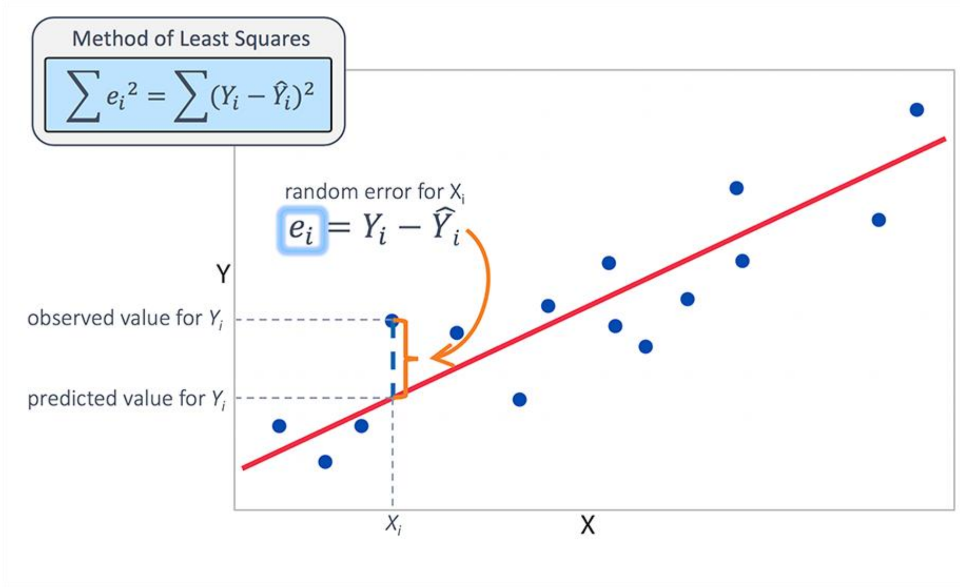
Equation 4-3. MSE cost function for a Linear Regression model

$$\text{MSE}\left(\mathbf{X}, h_{\boldsymbol{\theta}}\right) = \frac{1}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^{\intercal} \mathbf{x}^{(i)} - y^{(i)}\right)^2$$

Sometimes MAE is also used (less sensitive to outliers)

Equation 2-2. Mean absolute error (MAE)

$$\text{MAE}\left(\mathbf{X}, h\right) = \frac{1}{m} \sum_{i=1}^{m} \left| h\left(\mathbf{x}^{(i)}\right) - y^{(i)} \right|$$



Linear regression

- Make prediction by computing the weighted sum of features

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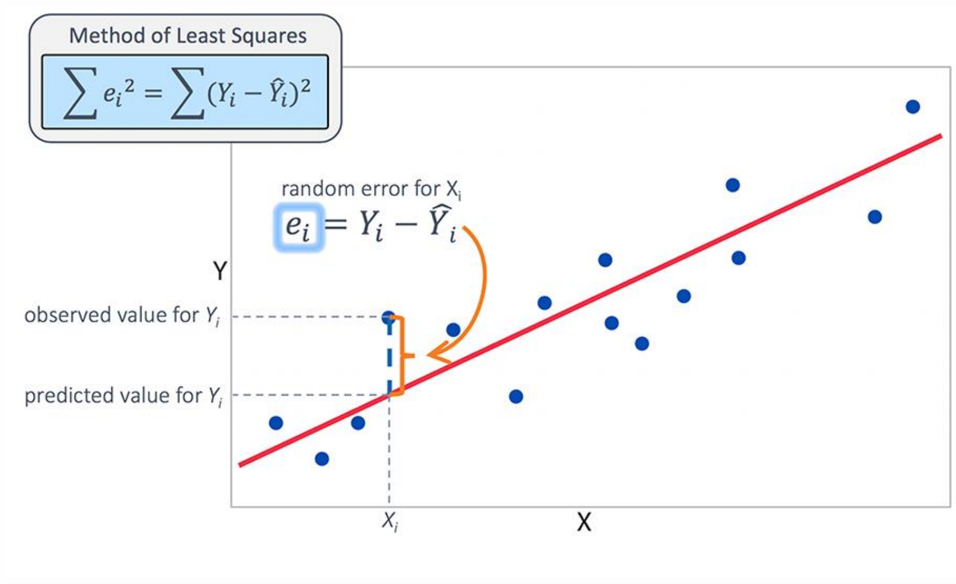
$$\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x}$$

- Train the model: find a parameter set to best fit the data

- Normal equation

$$\widehat{\boldsymbol{\theta}} = \left(\mathbf{X}^\intercal \mathbf{X}\right)^{-1} \mathbf{X}^\intercal \mathbf{y}$$

$$\boldsymbol{\theta} = E(\widehat{\boldsymbol{\theta}})$$



Polynomial regression

- When your data is more complex than a straight line
  - Add powers of a feature as new features

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2$$

Be aware of the combinatory explosion of features!

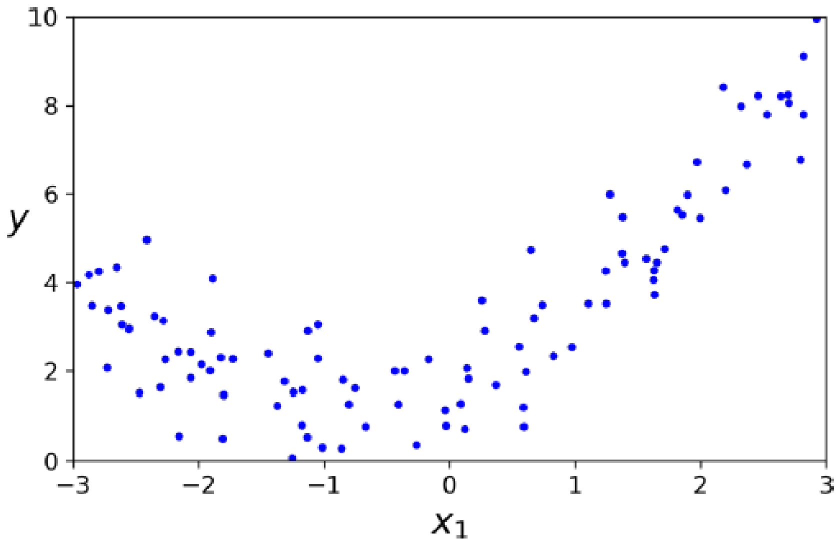
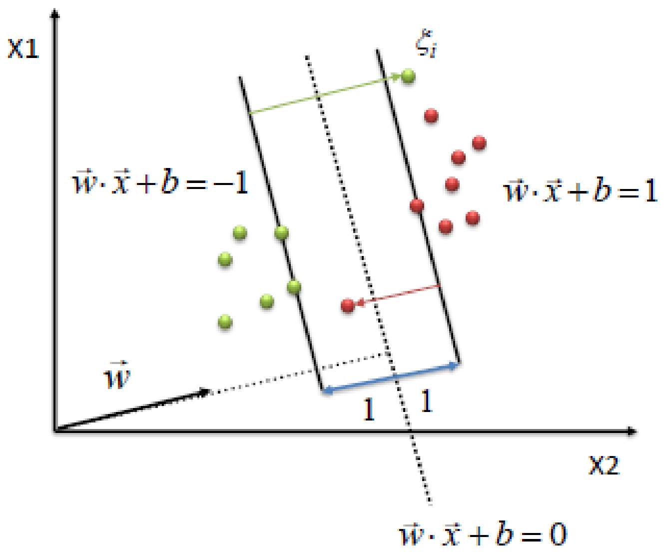


Figure 4-12. Generated nonlinear and noisy dataset

Support vector regression

SVM classification

fit the largest possible street between two classes while limiting margin violations



Constraint becomes :

$y_i(w\cdot x_i+b)\geq 1-\xi_i,\ \forall x_i$
$\xi_i \geq 0$

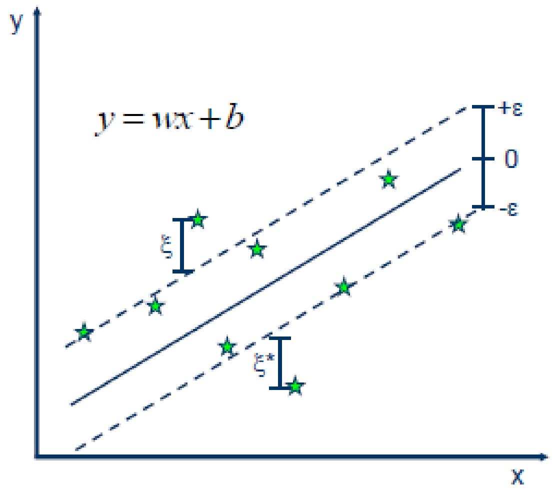
Objective function
penalizes for misclassified instances and those within the margin

$$\min \frac{1}{2}\|w\|^2 + C\sum_i \xi_i$$

C trades-off margin width and misclassifications

SVM regression

fit as many instances as possible *on* the street while limiting margin violations



- Minimize:

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\left(\xi_i+\xi_i^*\right)$$

- Constraints:

$$y_i - wx_i - b \leq \varepsilon + \xi_i$$
$$wx_i + b - y_i \leq \varepsilon + \xi_i^*$$
$$\xi_i, \xi_i^* \geq 0$$

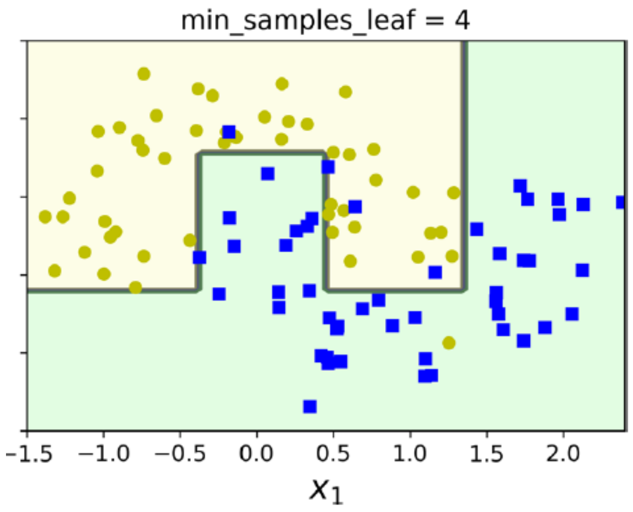
The kernel tricks can be used to solve nonlinear regression problem

http://www.saedsayad.com/support_vector_machine.htm

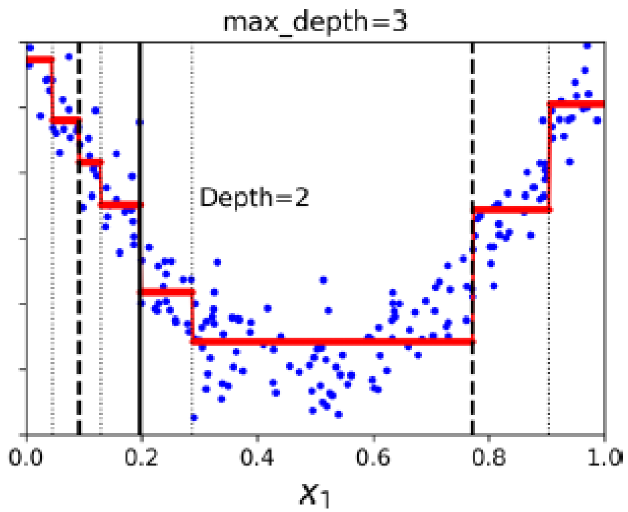
Tree-based regression

- The predicted value for each region is always the average target value of the instances in that region

Decision tree classification



Decision tree regression



Equation 6-4. CART cost function for regression

$$J(k, t_k) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \sum_{i\in\text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2 \\ \hat{y}_{\text{node}} = \dfrac{1}{m_{\text{node}}} \sum_{i\in\text{node}} y^{(i)} \end{cases}$$

Gradient Boosting Machines

Use decision trees as base-learner, iteratively improves the weak learning model

- Fit a decision tree to the data $\hat{y} = F_1(x)$
- Fit the next decision tree to the residuals from previous tree $h_1(x) = y - F_1(x)$
- Add the new tree to the algorithm $F_2(x) = F_1(x) + h_1(x)$
- Repeat this process until some mechanism tells us to stop (e.g. cross validation)

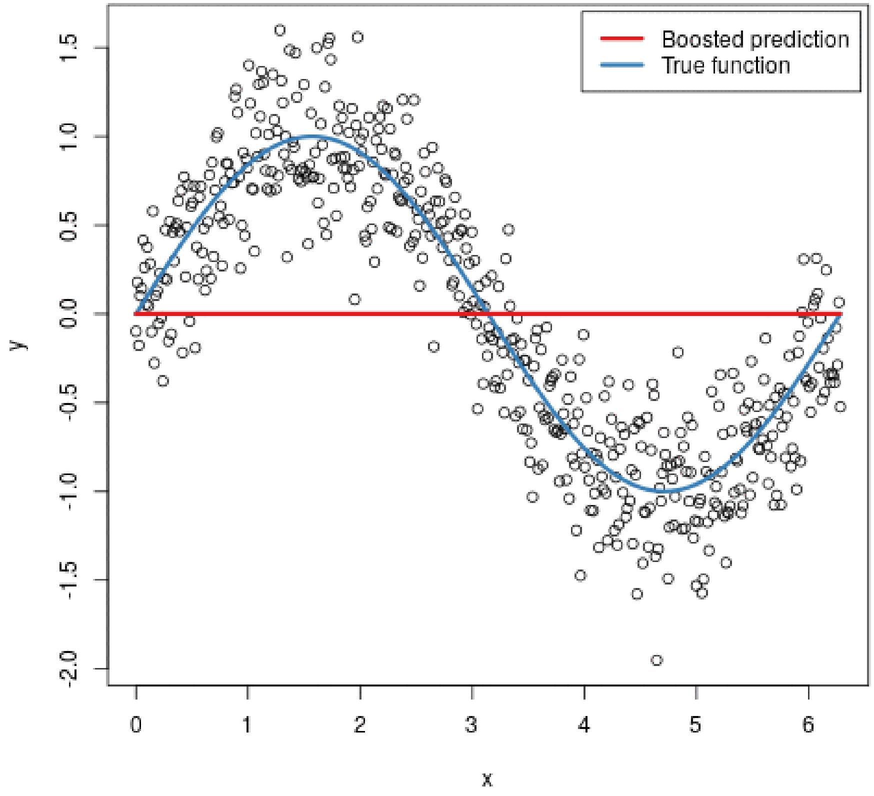
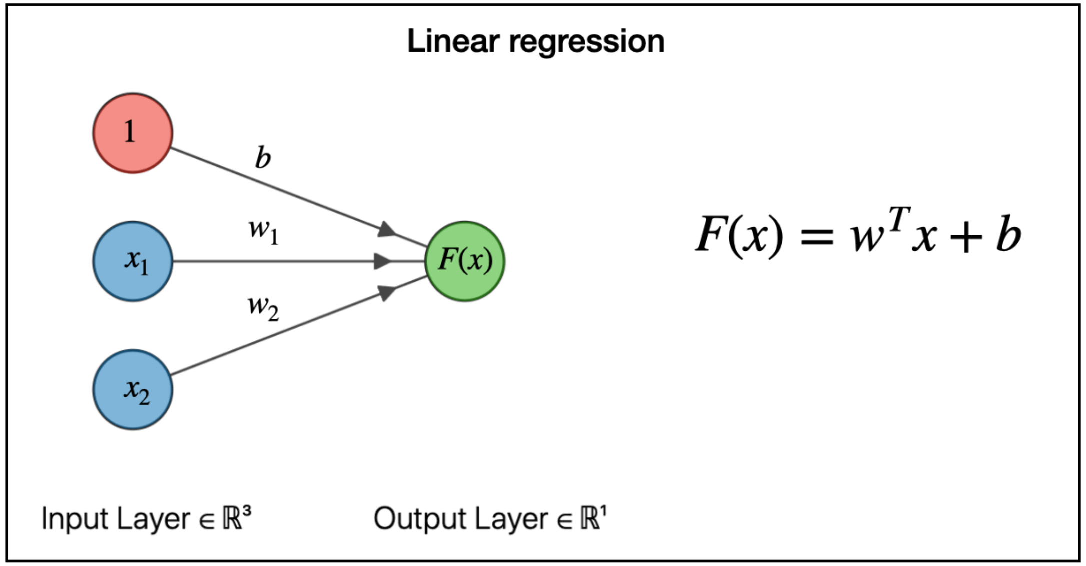
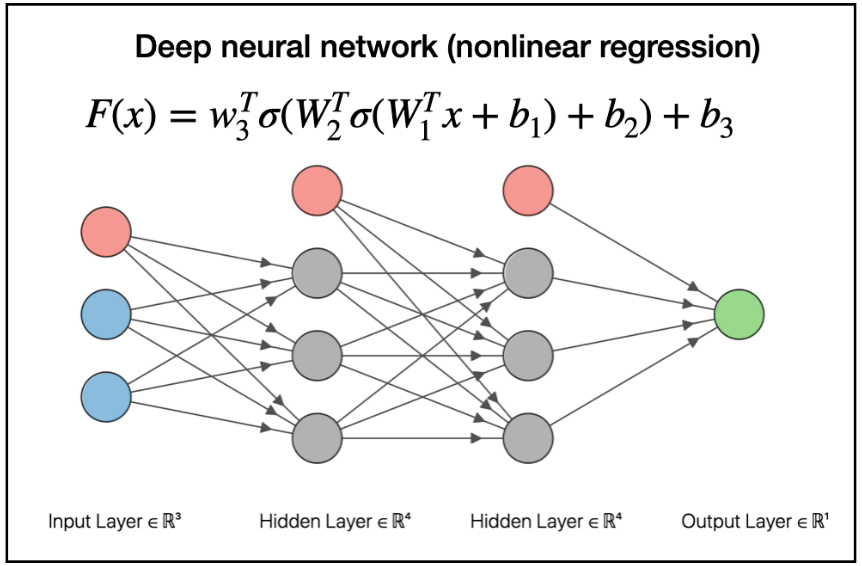


Image from internet

Neural Network

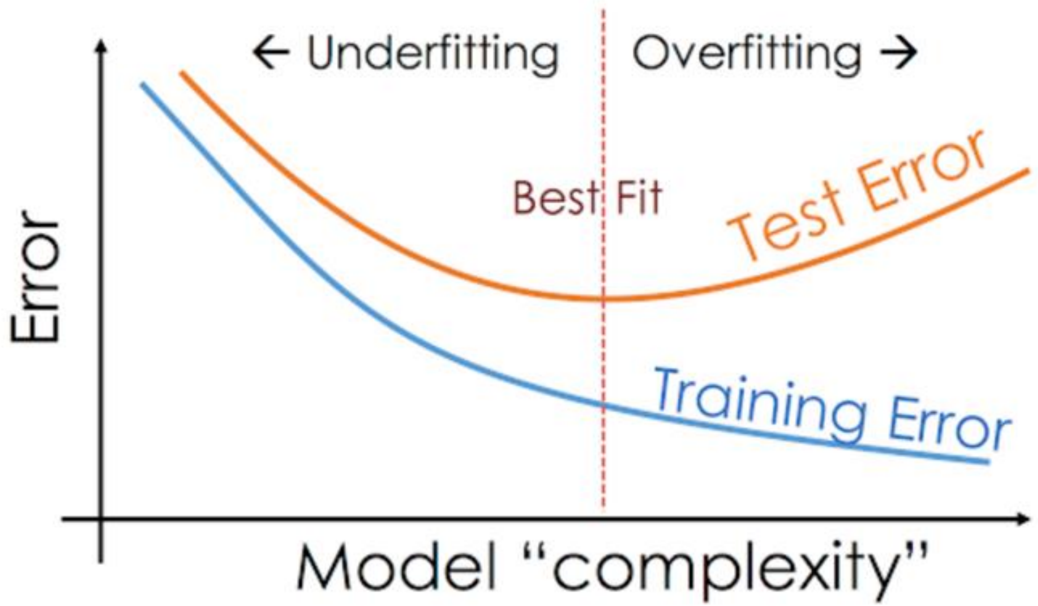
- A universal function approximator
  - Loss function: MSE
  - No sigmoid activation function at the output node





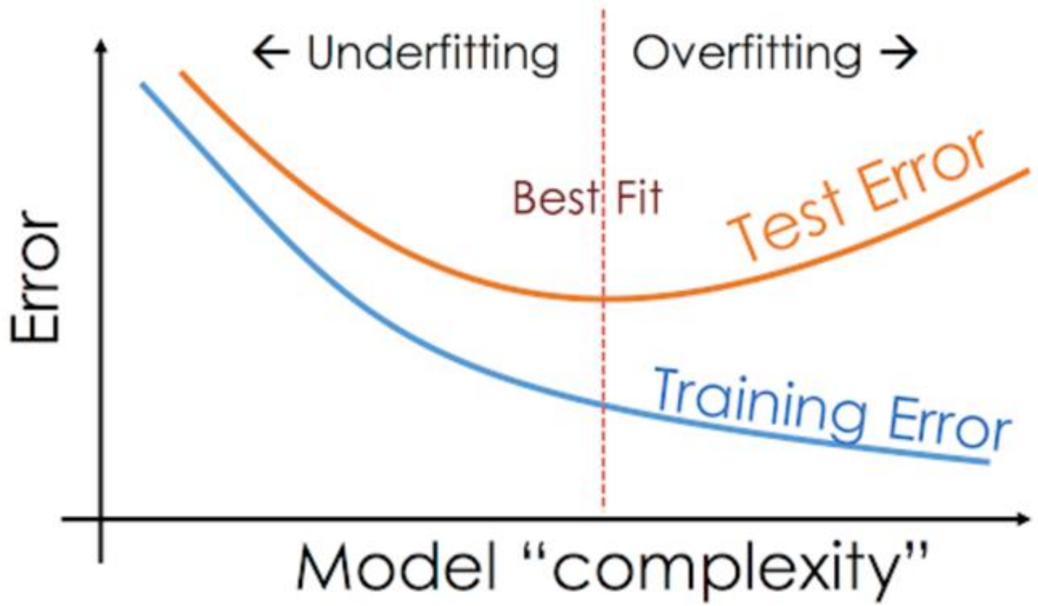
https://joshuagoings.com/2020/05/05/neural-network/

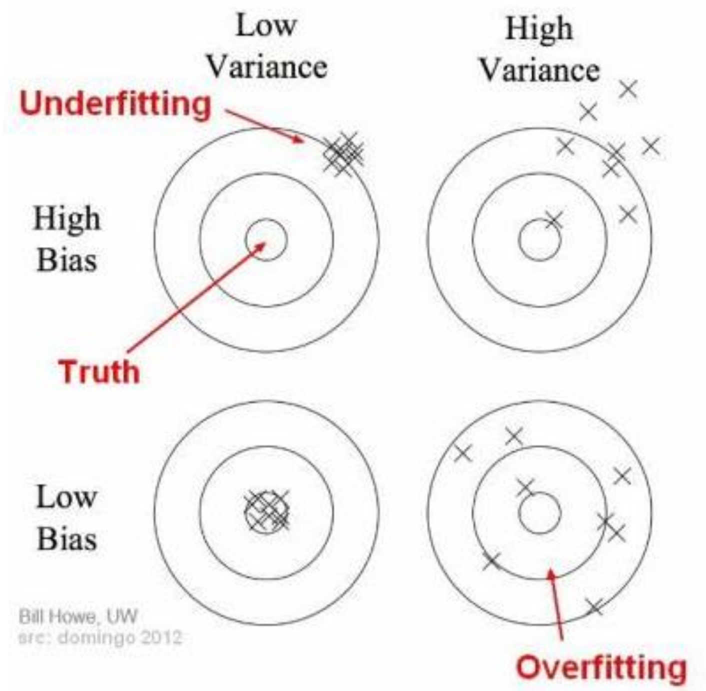
Over/underfit and bias-variance tradeoff



https://medium.com/@minions.k/underfit-and-overfit-explained-8161559b37db

Over/underfit and bias-variance tradeoff

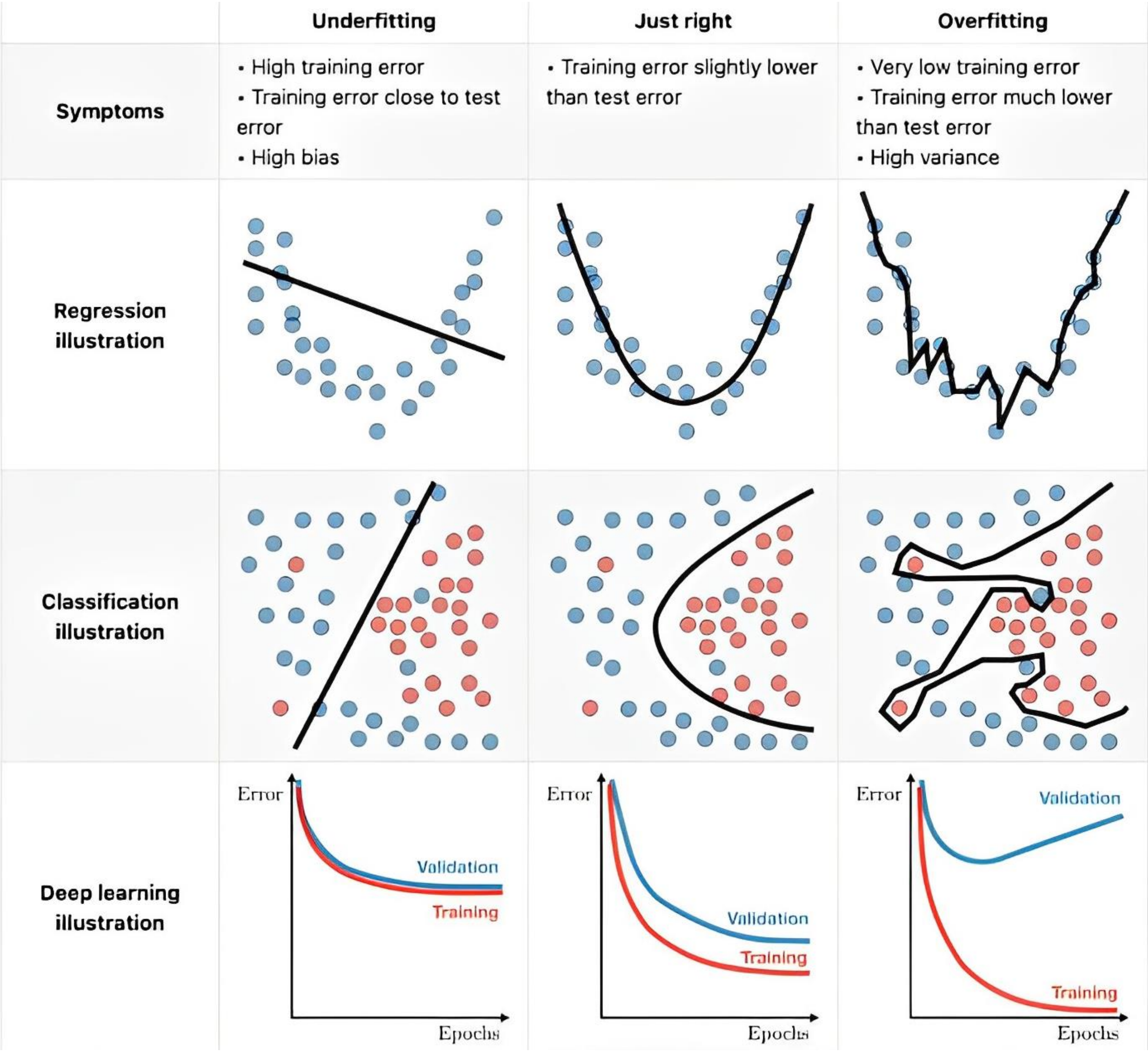




The bias-variance trade off

Underfit & Overfit

Symptom and solutions



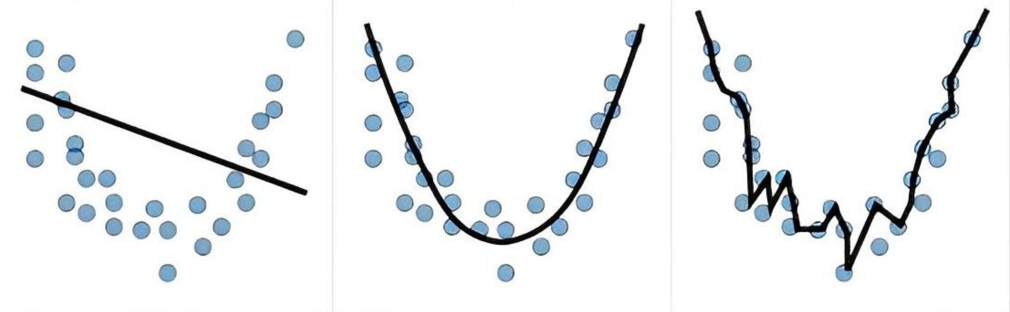
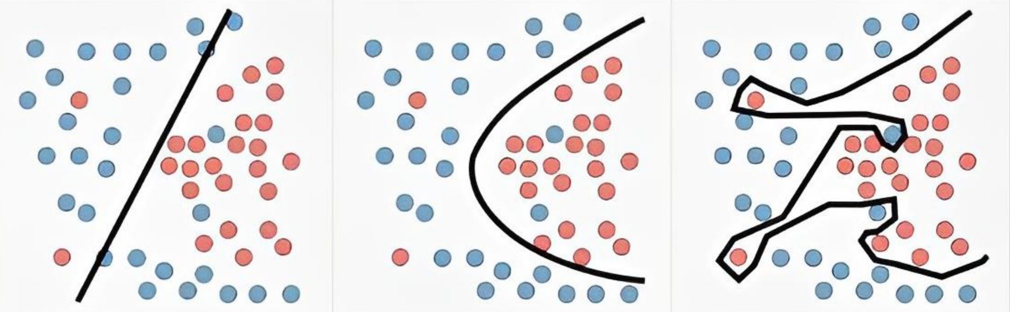
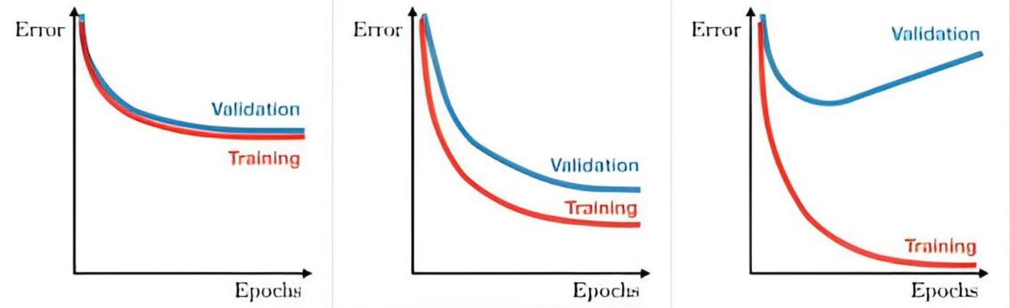
(too simple to explain the variance)

(forcefitting -- too good to be true)

https://www.kaggle.com/getting-started/180365

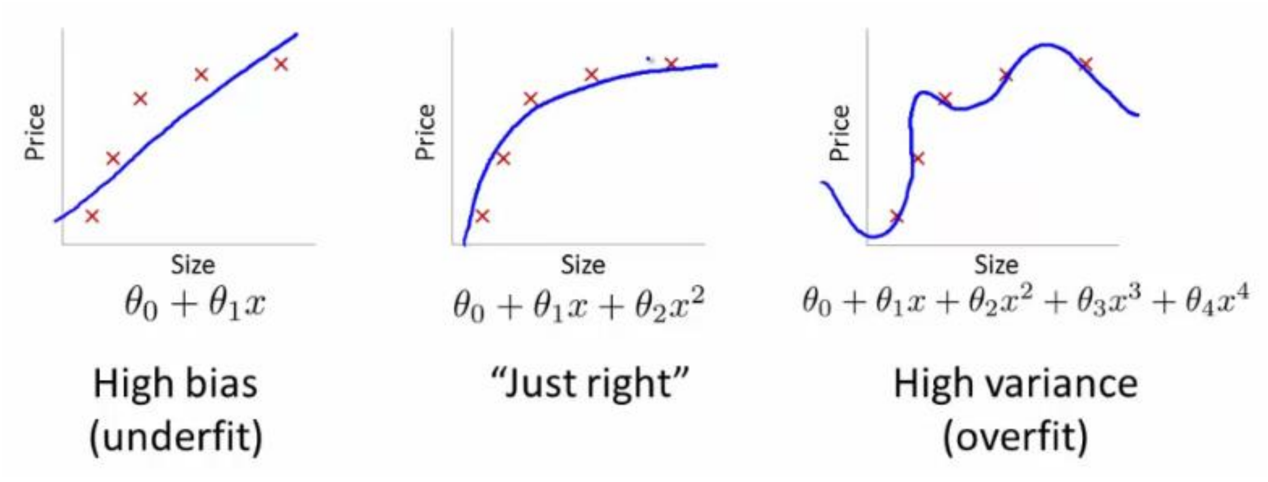
Underfit & Overfit

Symptom and solutions

	Underfitting	Just right	Overfitting
Symptoms	• High training error • Training error close to test error • High bias	• Training error slightly lower than test error	• Very low training error • Training error much lower than test error • High variance
Regression illustration			
Classification illustration			
Deep learning illustration			
Possible remedies	• Complexify model • Add more features • Train longer		• Perform regularization • Get more data

https://www.kaggle.com/getting-started/180365

Regularization techniques in regression



- Regularization: to put constrains on the model
  - The fewer degrees of freedom, the harder it overfits
  - In reality, it's common to have d >> n, regularization is usually needed

https://www.endtoend.ai/blog/bias-variance-tradeoff-in-reinforcement-learning/

3 typical constrains in regression

- Lasso (L1 penalty)

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + \alpha \sum_{i=1}^{n} |\theta_i|$$

- Ridge (L2 penalty)

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + \alpha \frac{1}{2} \sum_{i=1}^{n} {\theta_i}^2$$

This forces the learning algorithm to not only fit the data but also keep the model weights as small as possible!

- Elastic-net

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + r\alpha \sum_{i=1}^{n} |\theta_i| + \frac{1-r}{2} \alpha \sum_{i=1}^{n} {\theta_i}^2$$

3 typical constrains in regression

- Lasso (L1 penalty)

$$J(\boldsymbol{\theta}) = \mathrm{MSE}(\boldsymbol{\theta}) + \alpha \sum_{i=1}^{n} |\theta_i|$$

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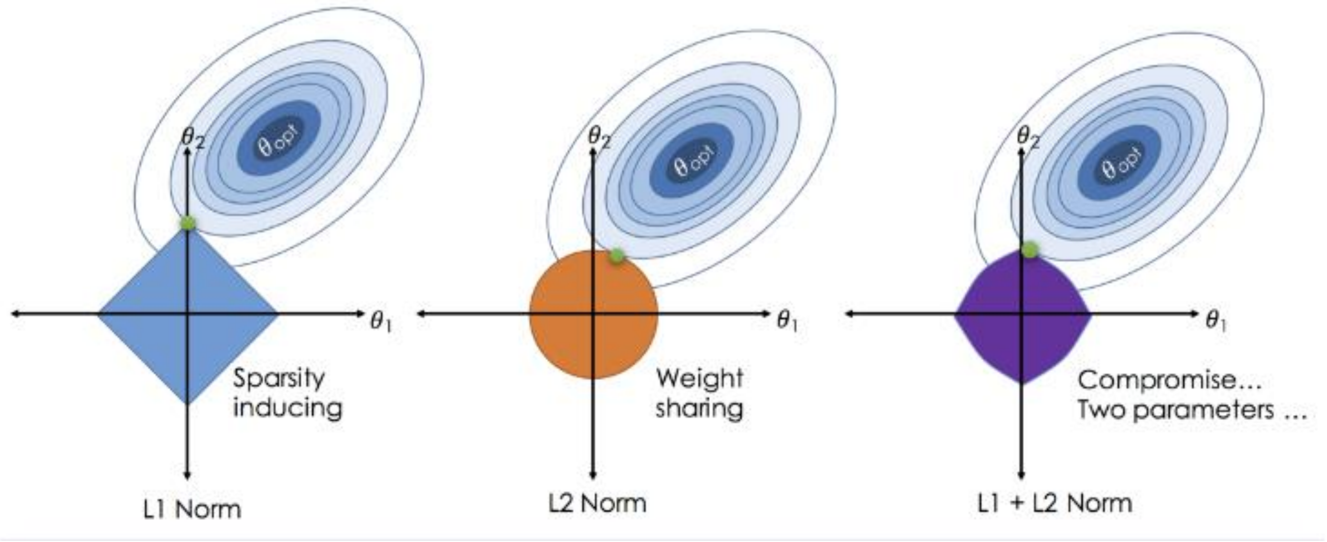


https://towardsdatascience.com/from-linear-regression-to-ridge-regression-the-lasso-and-the-elastic-net-4eaecaf5f7e6

Summary

- 6 regression algorithms
- MSE/MAE loss function
- Over/Underfit and Bias-variance tradeoff
- Regularization
  - LASSO
  - Ridge
  - Elastic net

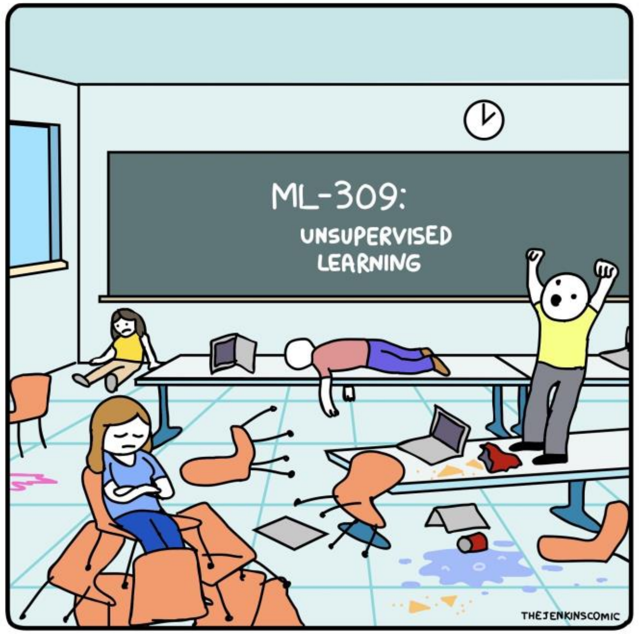
Unsupervised learning

- Dimension reduction
  - PCA
  - t-SNE
  - Autoencoder

  …

- Clustering
  - K-means
  - Hierarchical
  - DBSCAN

  …



Dimension reduction

- High dimensional: a blessing and a curse

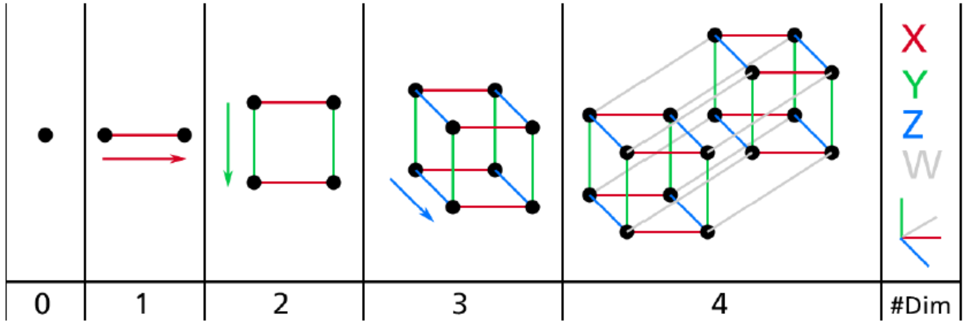


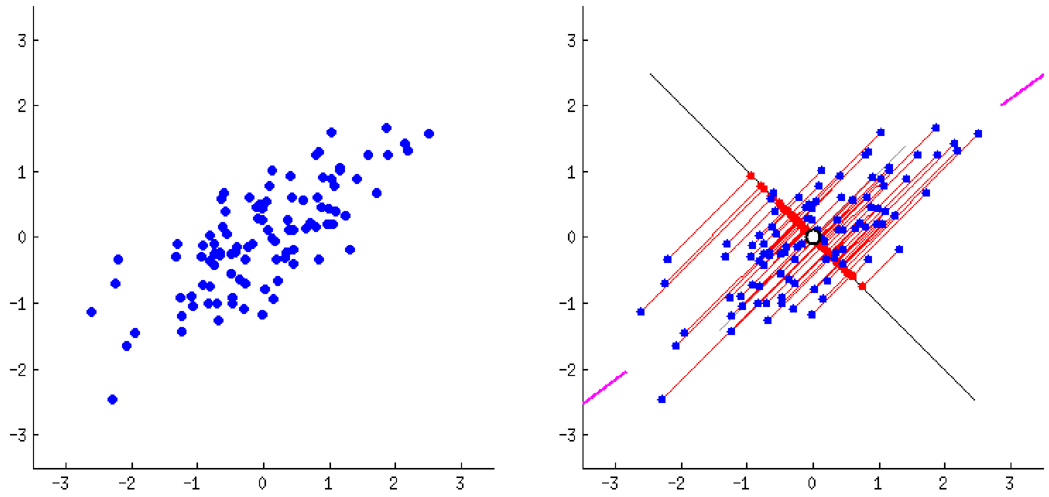
Figure 8-1. Point, segment, square, cube, and tesseract (0D to 4D hypercubes)[2]

- Curse of dimensionality:
  - Many machine learning algorithm have hard time to find good solutions in high dimensional setting
  - The training can be extremely slow when dimension (number of features) is high

Principal component analysis (PCA)

Preserving the maximum variance

- Data compression
- Noise removal
- Data visualization



https://sagarsaha455.medium.com/pca-for-visualization-and-dimension-reduction-14492e2acf2b

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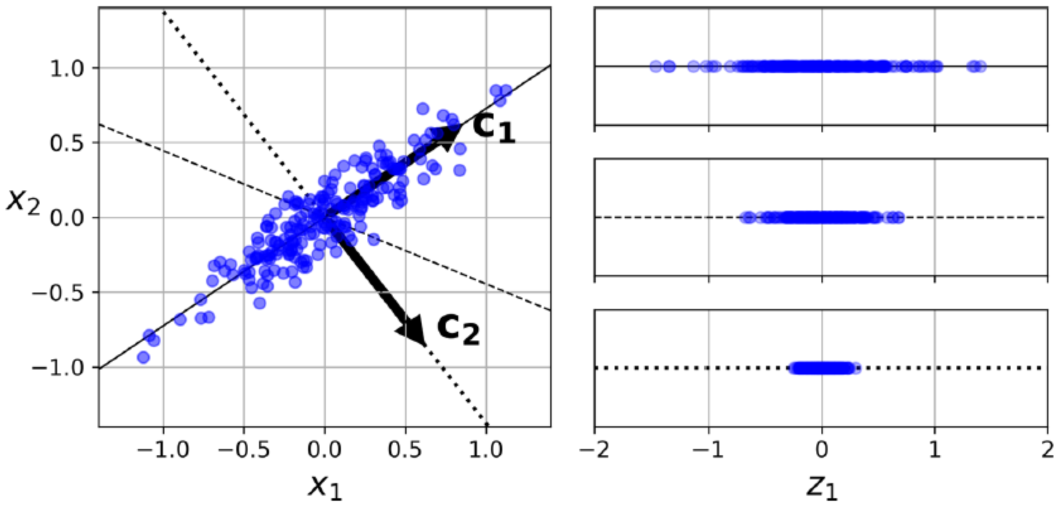

Figure 8-7. Selecting the subspace to project on

Principal component analysis (PCA)

Preserving the maximum variance
- Data compression
- Noise removal
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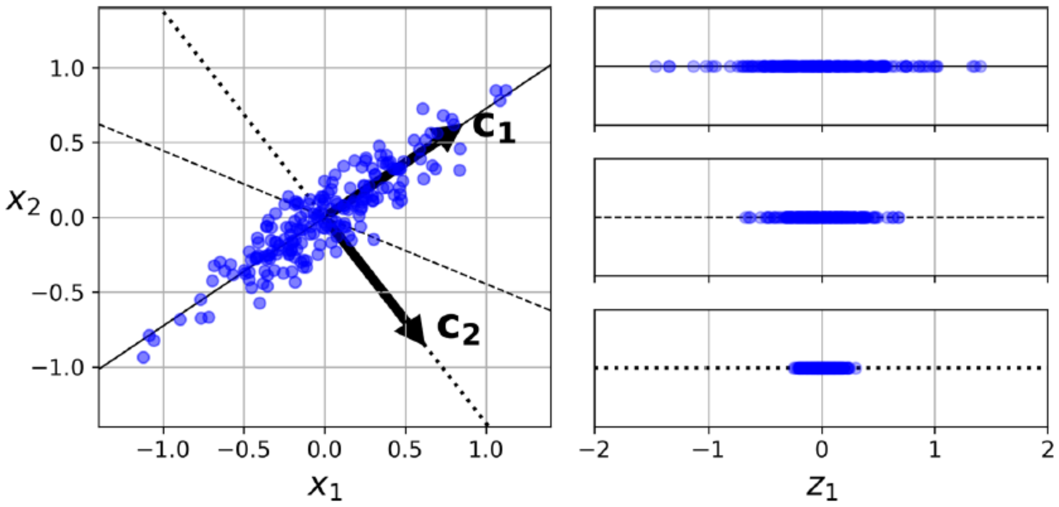


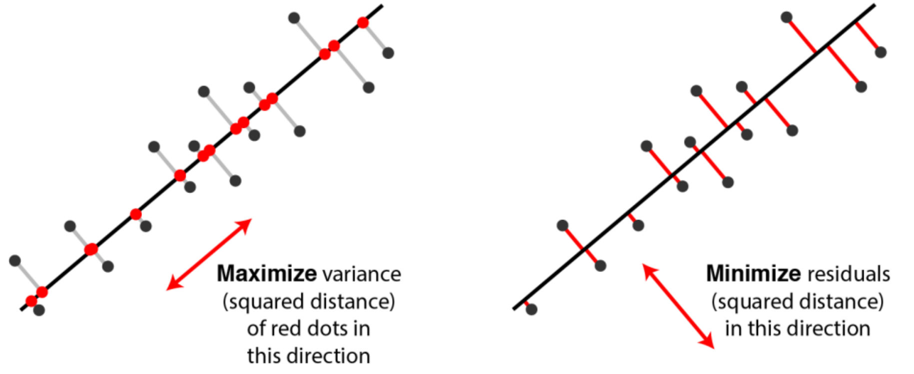
Figure 8-7. Selecting the subspace to project on

Goal:

- *find an orthogonal set of r linear basis vectors* $w_j \in R^d$ *and the corresponding score* $z_i \in R^r$*, such that we minimize the average* **reconstruction error**

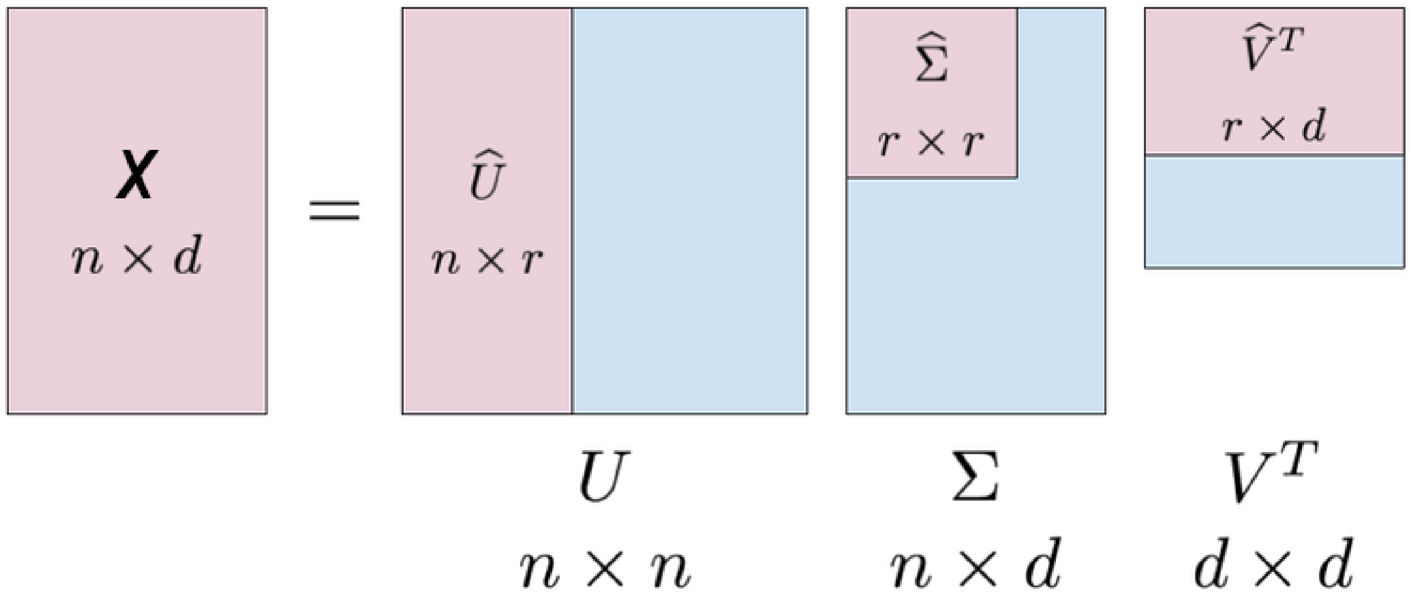
$$J(\mathbf{W}, \mathbf{Z}) = \frac{1}{N} \sum_{i=1}^{N} ||\mathbf{x}_i - \hat{\mathbf{x}}_i||^2$$

$$where\ \hat{\mathbf{x}}_i = \mathbf{W}\mathbf{z}_i$$



Principal component analysis (PCA)

- PCA achieved by Singular value decomposition (SVD)



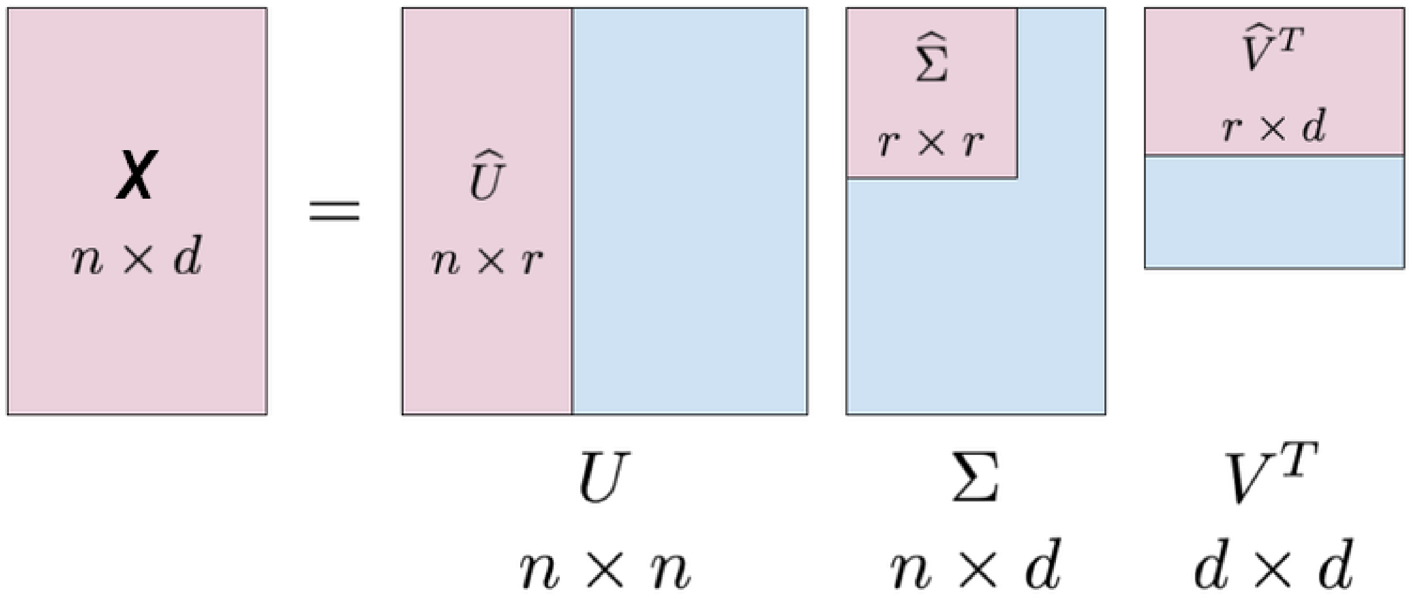
$\widehat{U}\,\widehat{\Sigma}$: Principal component scores

$\widehat{V}$: Principal directions

https://intoli.com/blog/pca-and-svd/

Principal component analysis (PCA)

- PCA achieved by Singular value decomposition (SVD)



- Project data on to the reduced dimension space

$$\boldsymbol{X}_{d-proj} = \boldsymbol{X}\widehat{\boldsymbol{V}}$$

https://intoli.com/blog/pca-and-svd/

t-Distributed Stochastic Neighbor Embedding (t-SNE)

- Nonlinear dimensionality reduction
  - PCA uses the global covariance matrix
  - t-SNE focus more on the local structure

- Core algorithm
  - In high dimensional space

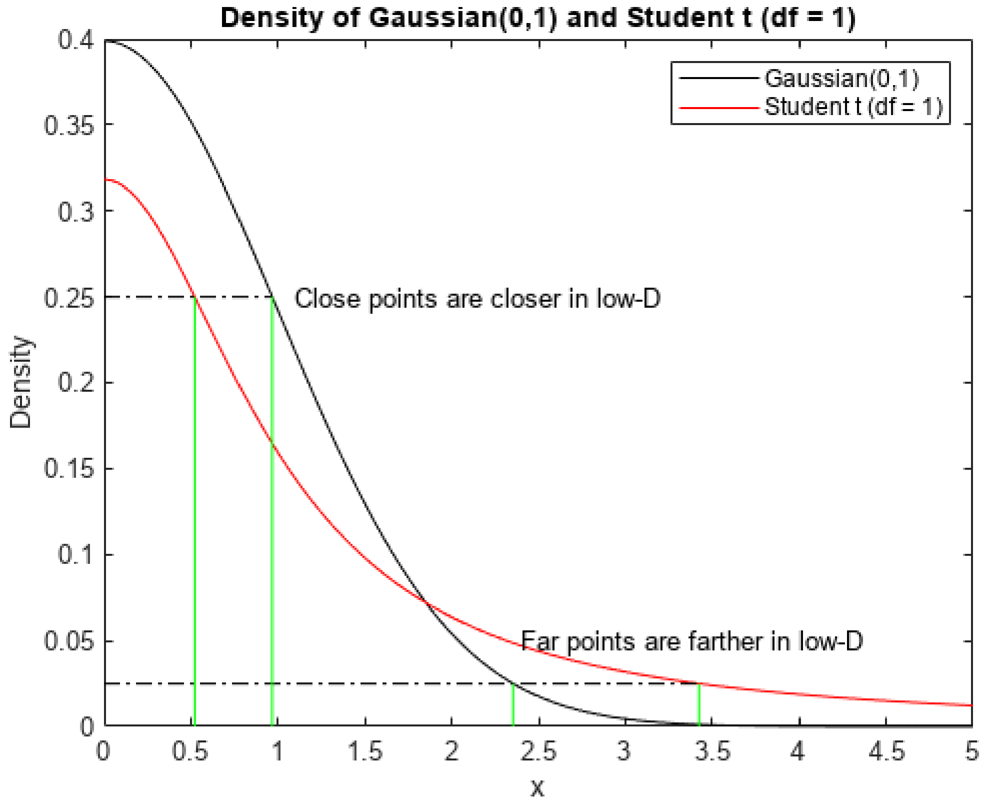
$$p_{ij} = \frac{\exp(-\left\|x_i - x_j\right\|^2 / 2\sigma_i^2)}{\sum_{k \neq l} \exp(-\left\|x_k - x_l\right\|^2 / 2\sigma_i^2)}$$

  - In lower dimensional space

$$q_{ij} = \frac{(1 + \left\|y_i - y_j\right\|^2)^{-1}}{\sum_{k \neq l}(1 + \left\|y_k - y_l\right\|^2)^{-1}}$$

  - Try to minimize the difference of 2 distributions

$$C = D_{\mathrm{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$



https://www.mathworks.com/help/stats/t-sne.html

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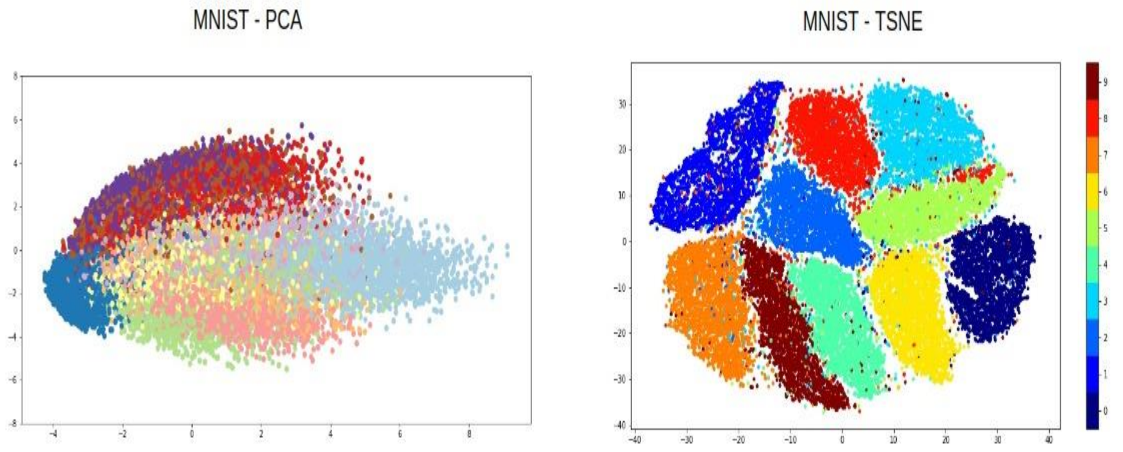

- Core algorithm
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  - Try to minimize the difference of 2 distributions

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Autoencoder

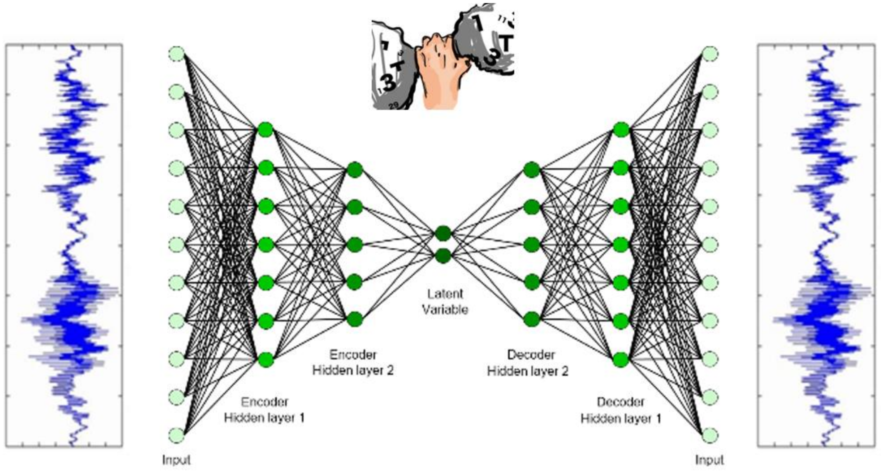
- Nonlinear dimension reduction with NN

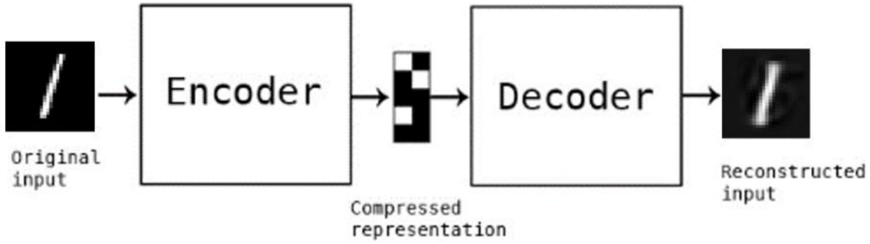
https://i-systems.github.io/teaching/ML/iNotes/15_Autoencoder.html

Autoencoder

- Nonlinear dimension reduction with NN

- Key idea:
  - An encoder function $z = f(x)$
  - A Decoder function $x = g(z)$
  - Learn to set $g\big(f(x)\big) \cong x$





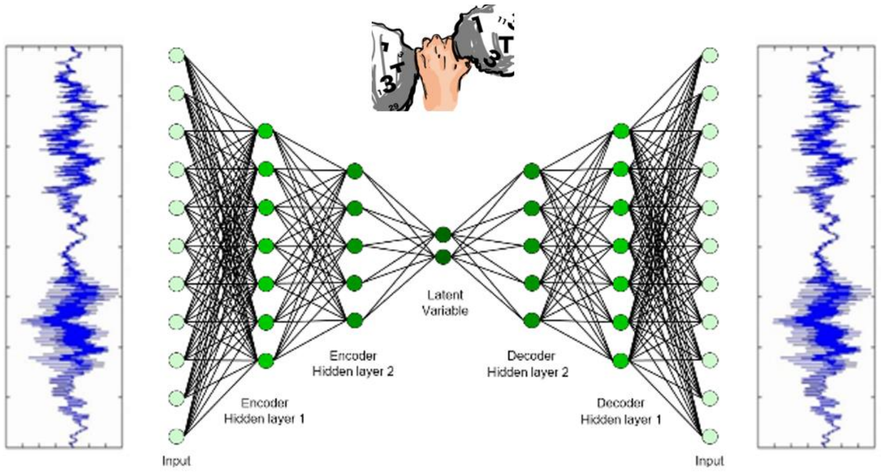
https://i-systems.github.io/teaching/ML/iNotes/15_Autoencoder.html

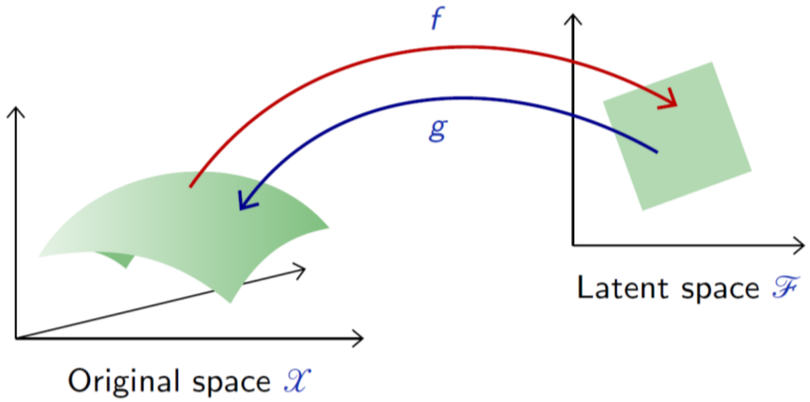
Autoencoder

- Nonlinear dimension reduction with NN

- Key idea:
  - An encoder function $z = f(x)$
  - A Decoder function $x = g(z)$
  - Learn to set $g\big(f(x)\big) \cong x$

- Loss function: reconstruction error
  - Minimize $||X - g \circ f(X)||^2$





https://i-systems.github.io/teaching/ML/iNotes/15_Autoencoder.html

Clustering

The vast majority of data is unlabeled. The clustering algorithm tries to identify similar instances and assigning them to *clusters*

- K-means
- Hierarchical clustering
- DBSCAN

Image from internet

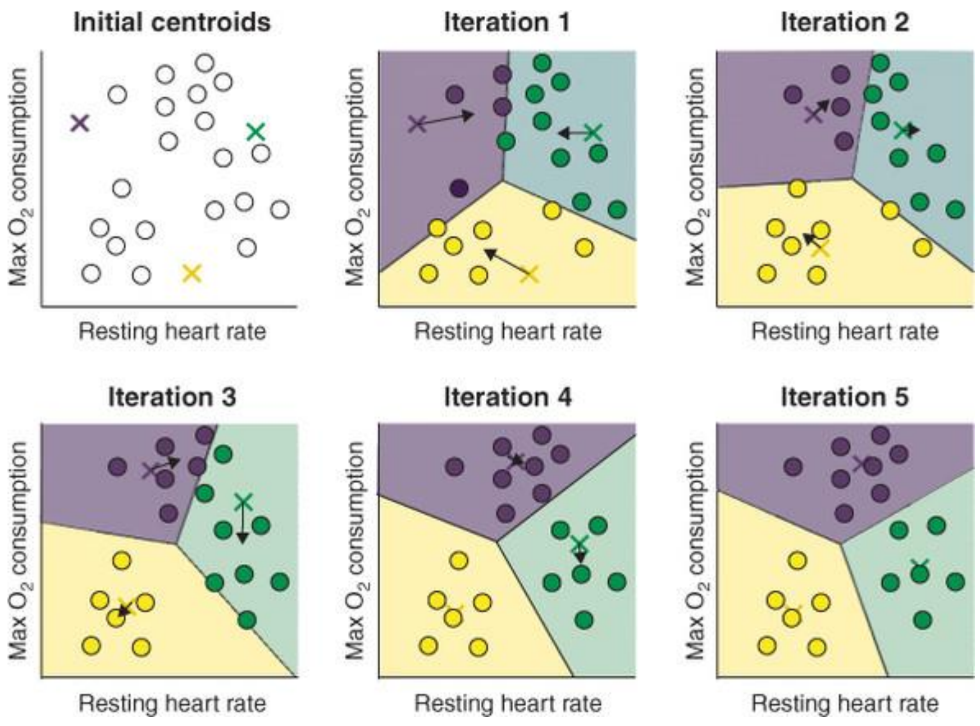
K-means

- Look for instances centered around a particular point (centroid)

- Core algorithm

Algorithm 1 k-means algorithm

1: Specify the number k of clusters to assign.
2: Randomly initialize k centroids.
3: **repeat**
4: **expectation:** Assign each point to its closest centroid.
5: **maximization:** Compute the new centroid (mean) of each cluster.
6: **until** The centroid positions do not change.



https://pub.towardsai.net/k-means-clustering-from-scratch-4e357ac4716f

K-means

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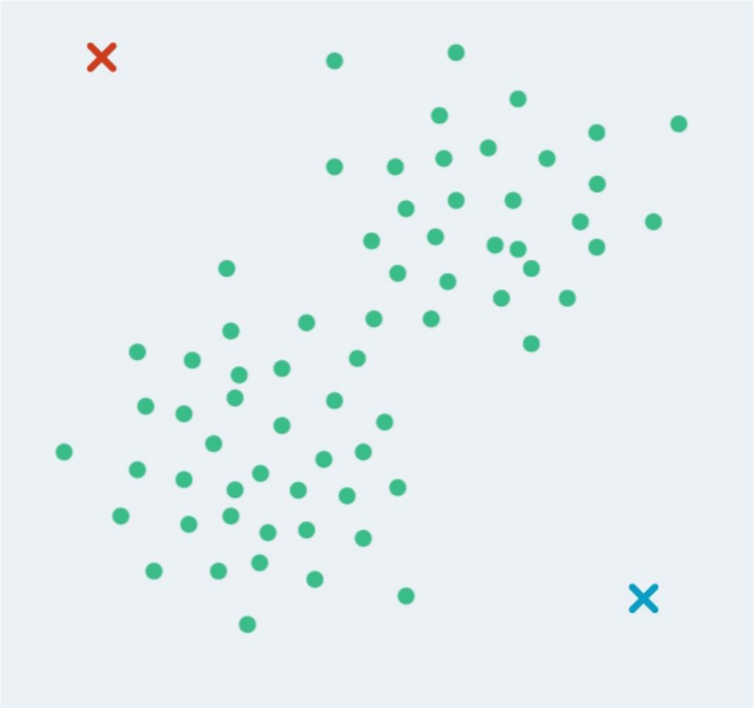

The algorithm is guaranteed to converge in a finite number of steps (usually quite small).

K-means

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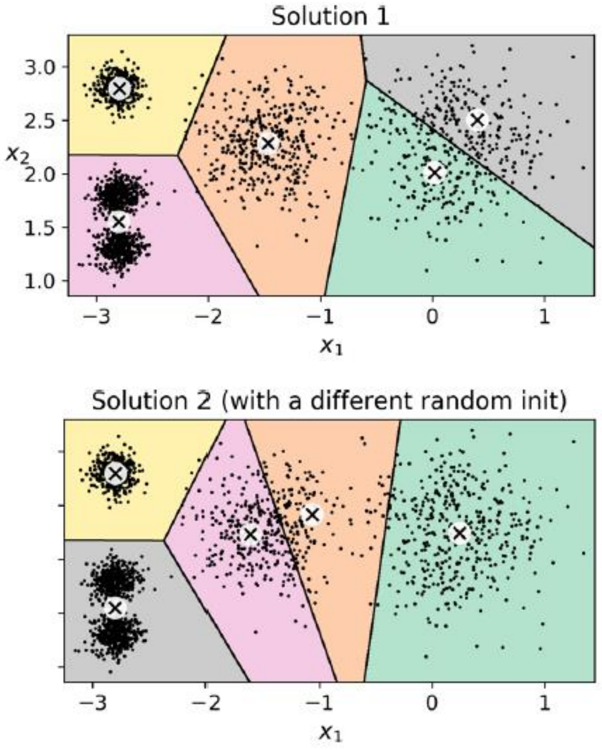

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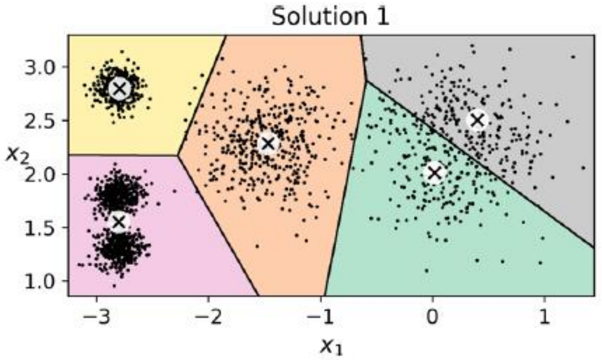

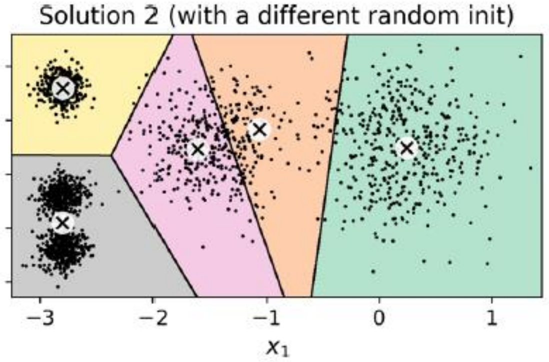

The algorithm is guaranteed to converge in a finite number of steps (usually quite small). But it might not converge to a right solution (local optimum)

Solution:
- If you know the approximate position of centroids, manually set them during initialization
- Run the algorithm multiple times with different random initialization, keep the best solution

K-means

- Look for instances centered around a particular point (centroid)

- Core algorithm

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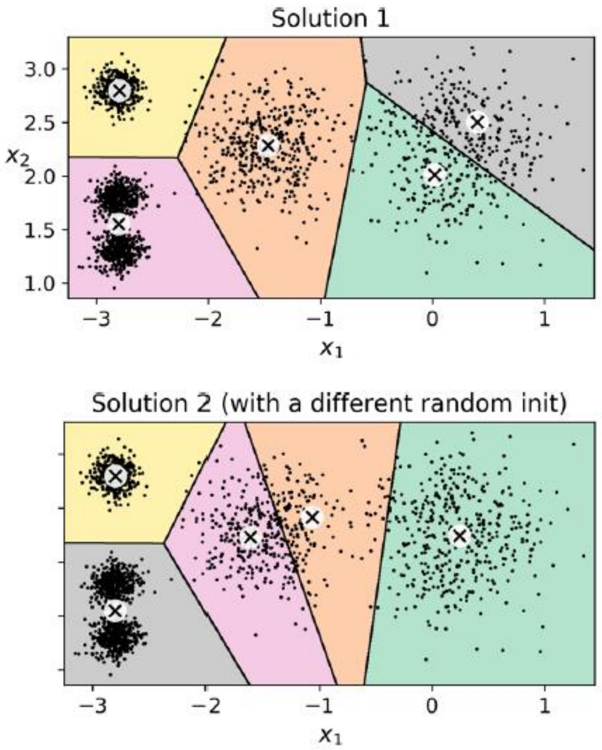


The algorithm is guaranteed to converge in a finite number of steps (usually quite small). But it might not converge to a right solution (local optimum)

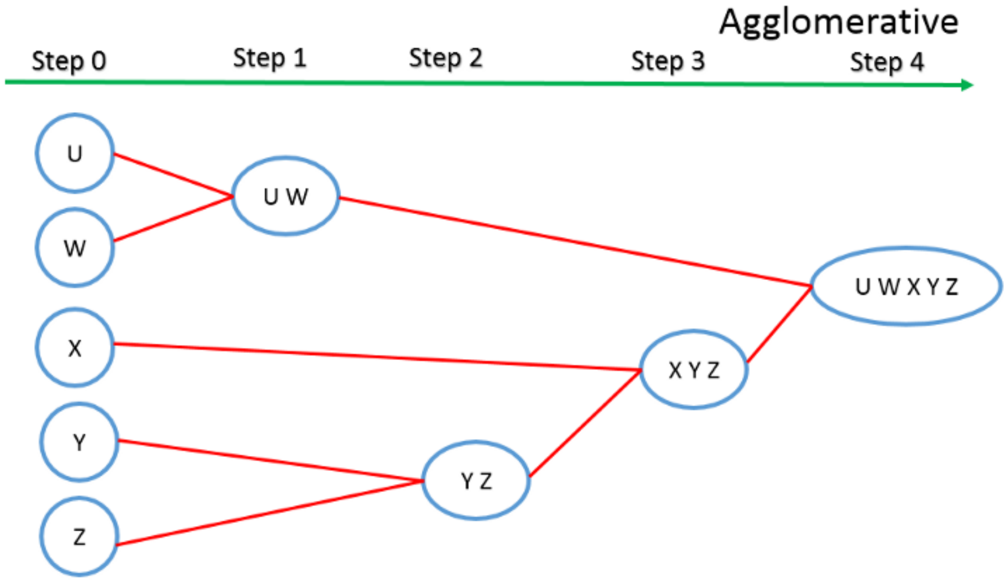
Note:

- K-means favor cluster with similar size, it doesn't perform well with varying sizes
- Need to specify the number of clusters

Hierarchical (Agglomerative) clustering

- A bottom-Up approach to connect the nearest pair of clusters

$t = 0$
Choose $R_0 = [C_i = x_i, i = 1, \ldots, N]$ as initial clustering
Repeat
  $t = t + 1$
  Find the closest clusters C_i, C_j in the existing clustering R_{t-1} such that
    $g(C_i, C_j) = \max_{r,s}(C_r, C_s)$ if g is similarity function
    $g(C_i, C_j) = \min_{r,s}(C_r, C_s)$ if g is dissimilarity function
  Define $C_q = C_i \cup C_j$ and produce the new clustering $R_t = [R_{t-1} - C_i - C_j] \cup C_q$
Until only one cluster is left



Hierarchical (Agglomerative) clustering

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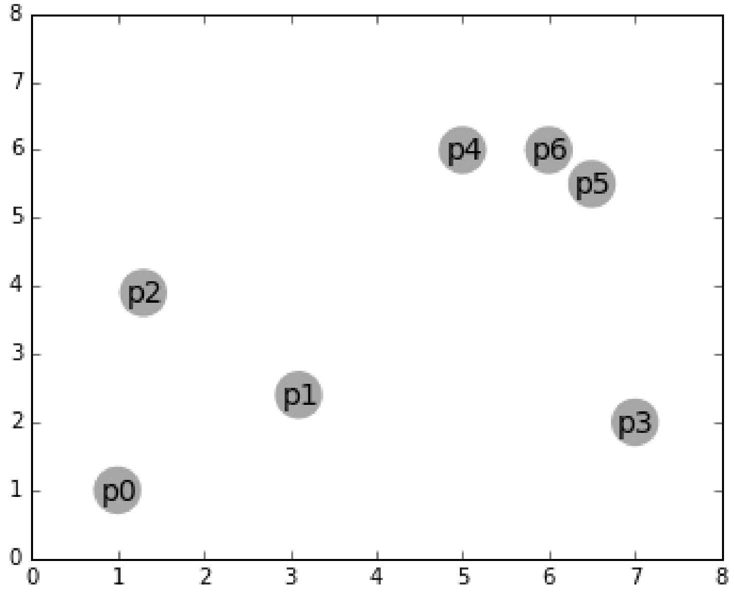
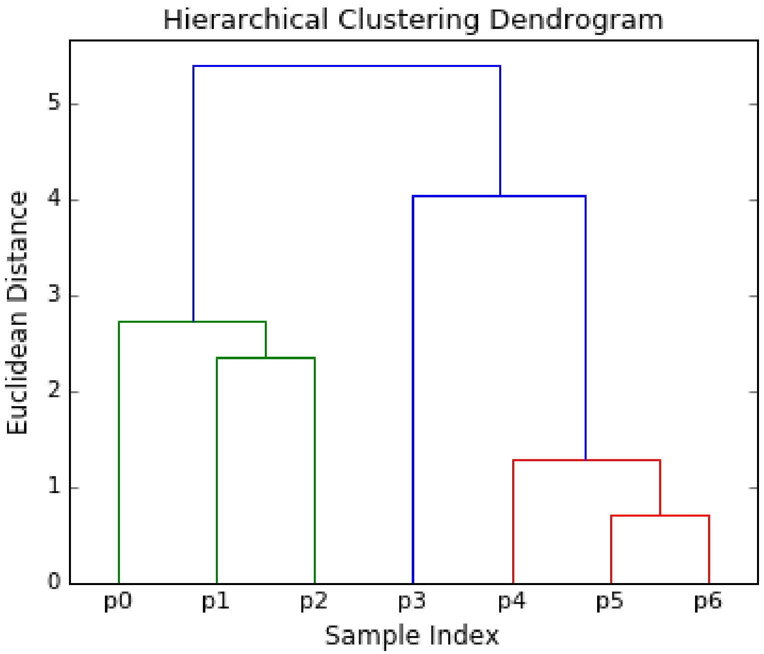




Scale up well to large number of instance or clusters

DBSCAN

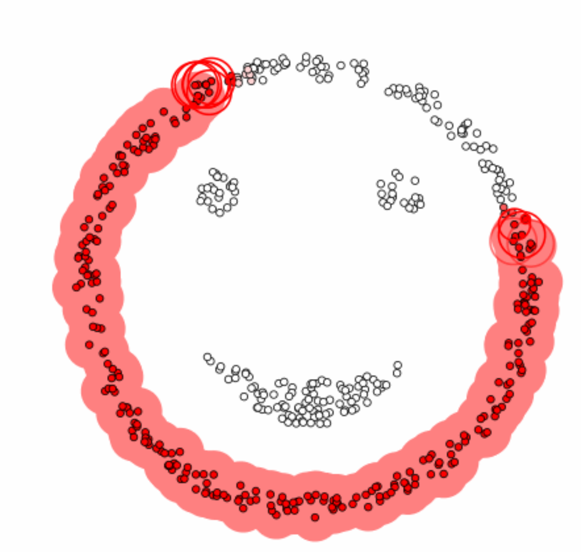
- Defines clusters as continuous regions of high density

- Core algorithm

Algorithm 3 : DBSCAN Clustering

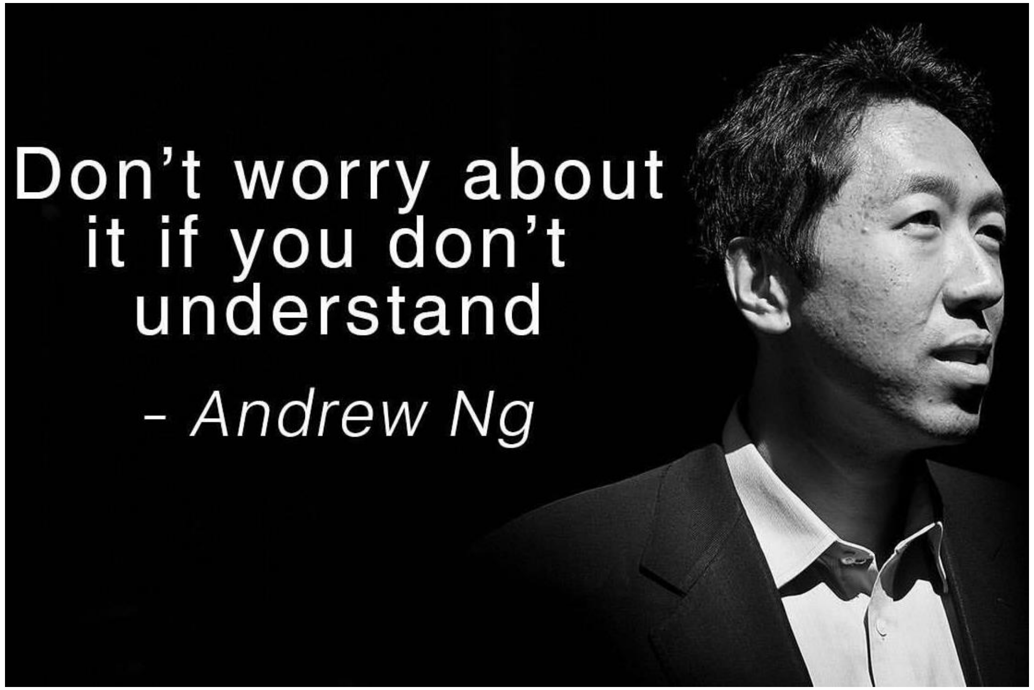
Input: 2*D_Data* obtained by *Algorithm1* as the input data, |Data| objects to be clustered, the neighborhood radius (ε) and minimum points (μ)

1: Randomly select a point *P*
2: Retrieve all points density-reachable from *P* based on ε and μ and Similarity Metric (*Algorithm2*)
3: If *P* is a core point, a cluster is formed.
4: If *P* is a border point, no points are density-reachable from P and DBSCAN selects the next no-visited point randomly.
5: Continue the procedure until all points have been processed.



- Works pretty well if clusters are dense enough and separated well by low-density regions
- Robust to outliers
- Computation complexity is $O(m \log m)$

Let’s do some practice!



➢ `git clone https://github.com/wbvguo/qcbio-ML_w_Python.git`

Summary

We have knowledge about

- ❑ Machine learning’s definition and categories
- ❑ The workflow for train a machine learning model
- ❑ Rationale of several major machine learning algorithms!
- ❑ Performance measure for evaluating models
- ❑ Challenges in machine learning and potential solutions

And we have experience in

- ❑ Jupyter notebook
- ❑ NumPy, matplotlib, scikit-learn, keras
- ❑ Build, train, evaluate a classifier or regressor
- ❑ Tune hyperparameters
- ❑ Unsupervised learning (PCA, K-Means)

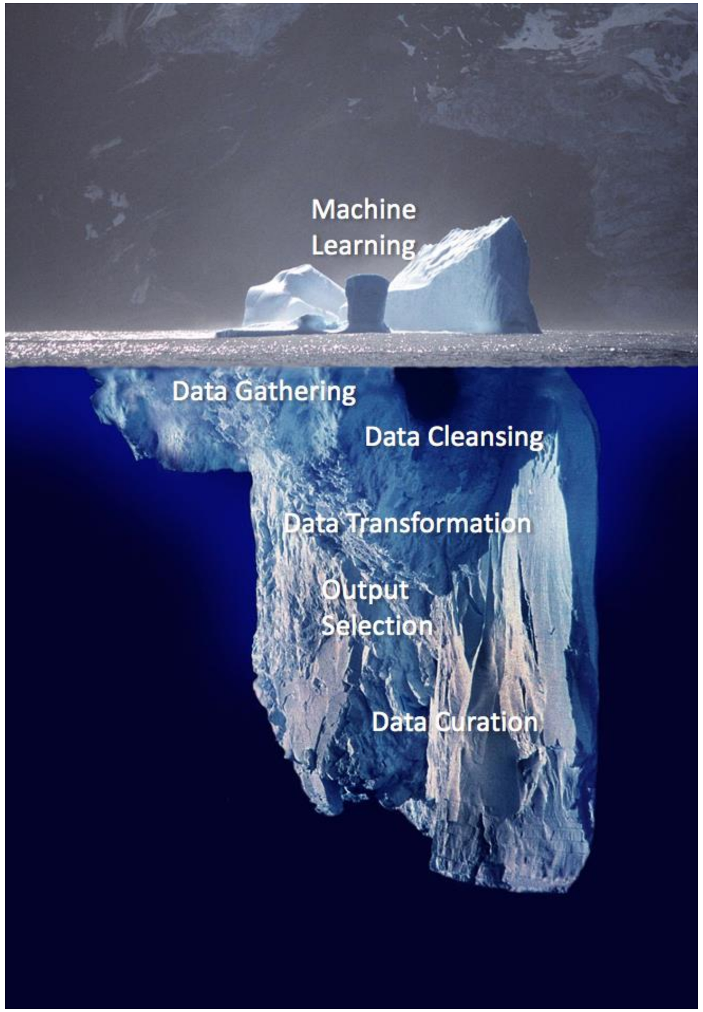
Summary of algorithms

Supervised learning		**Unsupervised learning**	
Classification	Regression	Dimension reduction	Clustering
Logistic regression	Linear regression	PCA	K-means
KNN	Polynomial regression	t-SNE	Hierarchical
Naïve bayes	SVR	Autoencoder	DBSCAN
SVM	Tree-based		
Decision tree	GBM		
Random forest	Neural Network		
Adaboost			
Gradient boosting			
Neural network			

Beyond machine learning algorithms

- Problem formulation
- Data cleansing
- Feature engineering
  - Feature encoding
  - Imputation: Missing data handling
  - Transformation/Normalization/Standardization

    …



Where to get help?

- https://www.google.com
- https://stackoverflow.com
- https://stats.stackexchange.com/
- https://towardsdatascience.com/
- https://www.3blue1brown.com
- https://statquest.org/
- https://openai.com/blog/chatgpt/

Lastly, GLHF!

"good luck, have fun with machine learning"

W Wenbin × DALL·E
Human & AI

Figure is generated by DALLE powered by OpenAI

Q&A

[Google docs]