KSBi-BIML 2026

Bioinformatics & Machine Learning(BIML) Workshop for Life Scientists

생명정보학 & 머신러닝 워크샵 (온라인)

Dimensionality Reduction

이제근 _ 숭실대학교

KSBI KOREAN SOCIETY FOR BIOINFORMATICS | 한국생명정보학회

본 강의 자료는 한국생명정보학회가 주관하는 BIML 2026 워크샵을 목적으로
제작된 것으로 해당 목적 이외의 다른 용도로 사용할 수 없음을 분명하게 알립니다.

이를 다른 사람과 공유하거나 복제, 배포, 전송할 수 없으며 만약 이러한 사항을 위반할 경우
발생하는 **모든 법적 책임은 행위자 본인에게 있음**을 알립니다.

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Bioinformatics & Machine Learning (BIML) Workshop for Life Scientists

한국생명정보학회가 주최하는 BIML-2026 동계 Bioinformatics &Machine Learning 교육 워크숍에 여러분을 초대합니다.

BIML 워크숍은 생명정보학 연구자들이 최신 AI바이오 분야의 인공지능 기반 분석 기술과 바이오 데이터 분석 기법을 이론과 실습을 통해 체계적으로 배울 수 있는 전문 교육 프로그램입니다. 2015년에 시작된 BIML 워크숍은 올해로 12년 차를 맞이하며, 국내 생명정보학 분야의 최초이자 최고 수준의 교육 프로그램으로 자리 잡았습니다. 이번 워크숍은 크게 인공지능바이오(AI바이오) 분야와 디지털바이오 분야, 두 분야로 구성됩니다.

AI바이오 분야에서는 생명정보 분석에 폭넓게 응용되고 있는 다양한 인공지능 기반 자료 모델링 기법을 다룰 예정입니다. 특히, 인공지능 심층학습을 활용한 단백질 구조 예측, 유전체 분석, 신약 개발에 대한 이론 및 실습 강의가 진행됩니다.

또한 디지털바이오 분야에서는 단일세포오믹스, 공간오믹스, 멀티오믹스, 메타오믹스에 대한 강의도 마련되어 있어, 연구자들의 분석 역량 강화에 실질적인 도움을 줄 것으로 기대됩니다.

또한 2024년부터 추가된 의료정보 자료 분석을 다루는 강의를 올해도 지속해서 운영하고자 합니다. 이는 최근 의료정보 자료 분석에 관한 연구 수요 증가를 반영한 것으로, 관련 연구를 수행하는 의과학자 및 의료정보 연구자들에게 유용한 지침을 제공할 것입니다.

또한, 올해도 생명정보학 기술의 다양화에 발맞춰 온라인 강좌를 대폭 확대했습니다. 올해는 무료 강좌 10개를 포함한 총 40개 이상의 강좌가 개설되며, 연구 주제에 맞는 강좌 추천과 강연료 할인 혜택도 제공합니다.

BIML-2026는 국내 주요 연구 중심 대학의 전임 교수 및 각 분야 최고 전문가들의 강의로 구성되어 있으며, 기초 이론부터 최신 연구 동향까지 아우르는 심도 있는 교육의 장이 될 것으로 확신합니다.

여러분의 많은 관심과 참여를 기대합니다!

2026년 2월

한국생명정보학회장 류 성 호

강의개요

Dimensionality Reduction

바이오 데이터는 고차원의 데이터로 구성되어 있는 경우가 많다. 일례로 유전자 발현 데이터를 생각하면, 일반적으로 유전자가 변수(feature)가 되기에 인간의 경우 20,000 차원의 이상으로 구성된 데이터라 할 수 있으며 이러한 고차원의 데이터를 이용하여 분석을 진행하는 것은 계산학적으로도 간단한 일이 아니다.

본 강의에서는 이러한 고차원 데이터를 분석할 때 활용할 수 있는 dimensionality reduction (차원 축소) 개념과 대표적인 방법들, 활용 방안에 대해 설명한다. 가장 대표적인 방법인 PCA (principal component analysis)를 비롯하여 ICA (independent component analysis), NMF (non-negative matrix factorization)등 여러 방법론에 대해 간단히 소개한다. 또한 deep neural networks을 이용하여 dimensionality reduction 목적으로 사용할 수 있는 autoencoder의 개념과 활용에 대해서도 설명한다. 각 방법들에 대한 기본 개념 소개와 함께 실제 데이터를 이용한 활용 예시를 통해 이러한 방법들이 바이오 데이터 분석에 어떻게 활용될 수 있는지 보인다.

본 강의에서는 수학적인 부분을 아예 제외할 수는 없으나, 각 방법의 특성을 비롯한 주요 개념 이해를 목적으로 설명한다. 또한 이론 위주의 강의이나 R이나 python을 이용하여 해당 방법들을 어떻게 활용할 수 있는지에 대해서도 간단히 소개한다. 직접적인 R이나 python 실습이 진행되지는 않지만, 강의 중 소개되는 코드 이해를 위해서는 R과 python 기초 문법을 사전에 알고 있으면 도움이 될 수 있다.

* 참고강의교재: 강의 자료

* 교육생준비물: 강의 수강을 위한 개인 컴퓨터

* 강의 난이도: 초급

* 강의: 이제근 교수 (숭실대학교 의생명시스템학부)

Curriculum Vitae

Speaker Name: Je-Keun Rhee, Ph.D.

▶ **Personal Info**

Name	Je-Keun Rhee
Title	Assistant Professor
Affiliation	Soongsil University

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Research Interest

Cancer Genomics, Machine Learning

Educational Experience

2004	B.S. in Life Science, Korea University, Korea
2004	B.S. in Computer Science & Engineering, Korea University, Korea (Double Major)
2014	Ph.D. in Bioinformatics, Seoul National University, Korea

Professional Experience

2011	Visiting Scholar, School of Informatics and Computing (SoIC), Indiana University, USA
2014-2018	Research Professor, Cancer Research Institute / Department of Medical Informatics, The Catholic University of Korea, Korea
2018-2019	Assistant Professor, School of Dentistry, Pusan National University, Korea
2019-	Assistant Professor, School of Systems Biomedical Sciences, Soongsil University, Korea

Selected Publications (5 maximum)

1. Bonil Koo, Je-Keun Rhee, Prediction of tumor purity from gene expression data using machine learning, Briefings in Bioinformatics, 22(6):bbab163, 2021. (Corresponding author)
2. Yeongjoo Kim, Ji Wan Kang, Junho Kang, Eun Jung Kwon, Mihyang Ha, Yoon Kyoung Kim, Hansong Lee, Je-Keun Rhee, Yun Hak Kim, Novel deep learning-based survival prediction for oral cancer by analyzing tumor-infiltrating lymphocyte profiles through CIBERSORT, OncoImmunology, 10(1):e1904573, 2021 (Co-corresponding author)
3. Joong Chae Na, Inbok Lee, Je-Keun Rhee, and Soo-Yong Shin, Fast single individual haplotyping method using GPGPU, Computers in Biology and Medicine, 113:103421, 2019. (Co-corresponding author)
4. Je-Keun Rhee, Soo-Jin Kim, Byoung-Tak Zhang, Identifying DNA Methylation Modules Associated with a Cancer by Probabilistic Evolutionary Learning , IEEE Computational Intelligence Magazine, 13(3): 12-19, 2018. (First author)
5. Joong Chae Na, Jong-Chan Lee, Je-Keun Rhee, and Soo-Yong Shin, PEATH: Single Individual Haplotyping by Probabilistic Evolutionary Algorithm with Toggling, Bioinformatics, 34(11): 1801-1807, 2018. (Co-corresponding author)

KSBi-BIML

Dimensionality Reduction

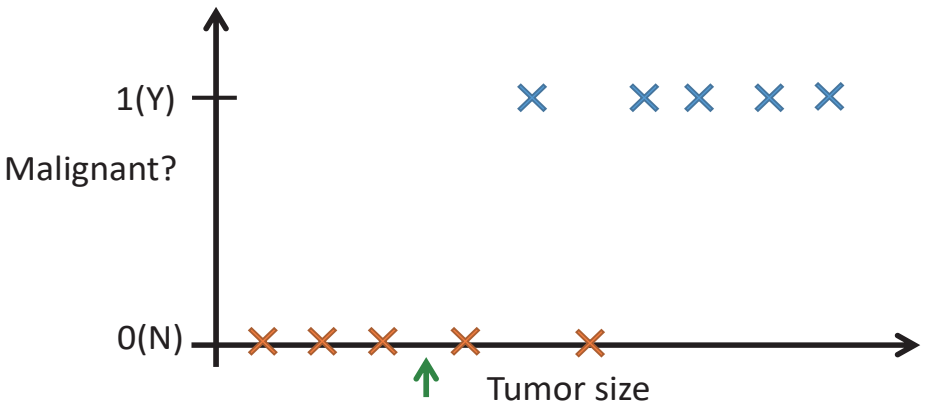
Rhee, Je-Keun

Soongsil University (숭실대 이제근)

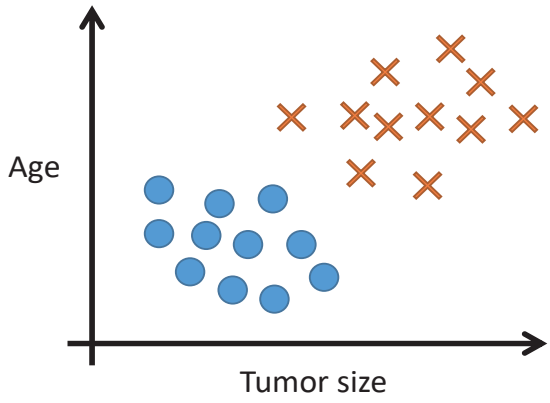
SBi 한국생명정보학회 Korean Society for Bioinformatics

Cancer (Malignant, Benign)

숭실대학교 Soongsil University

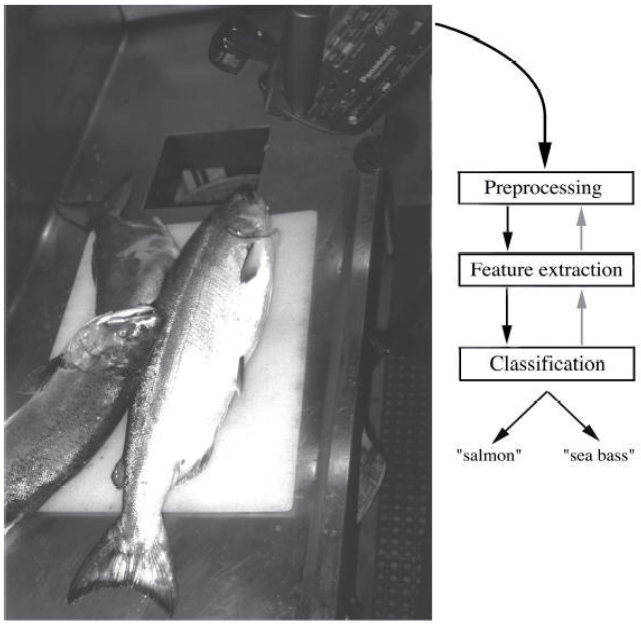


Cancer Classification



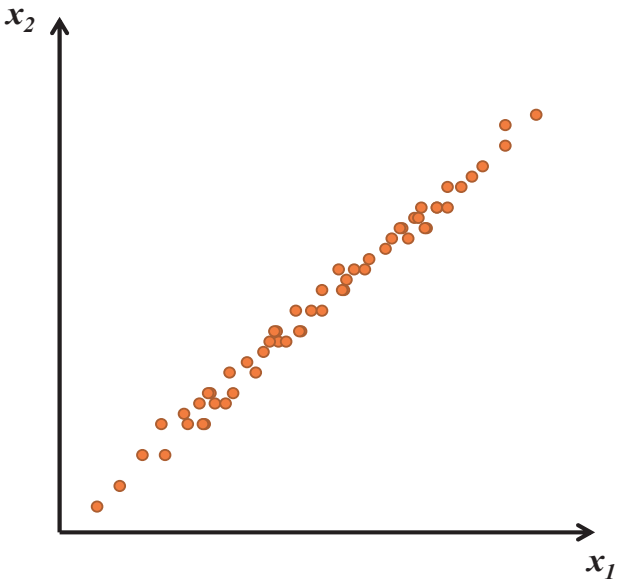
- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape
- …

Dimension Reduction / Feature Selection

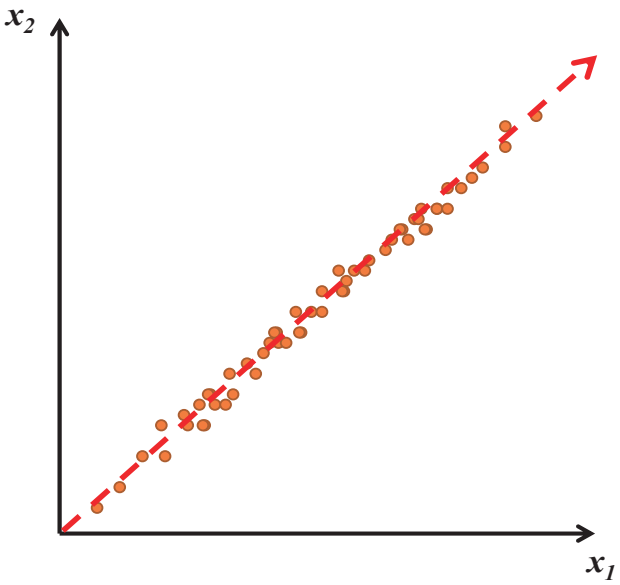


from Pattern Classification (book)

Principal component analysis (PCA)



(0.9, 1.0), (1.3, 1.4), (1.9, 1.8), (2.2, 2.2), (2.4, 2.3), ….



From *k* original variables: $x_1,x_2,\ldots,x_k$:

Produce *k* new variables: $y_1,y_2,\ldots,y_k$:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + \ldots + a_{2k}x_k$$
$$\ldots$$
$$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$$

y_k's are
Principal Components

such that:

y_k's are orthogonal
y_1 explains as much as possible of original variance in data set
y_2 explains as much as possible of remaining variance etc.

$\{a_{11},a_{12},...,a_{1k}\}$ is 1st **Eigenvector** of covariance matrix, and **coefficients** of first principal component

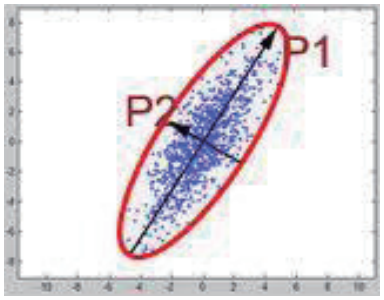
$\{a_{21},a_{22},...,a_{2k}\}$ is 2nd **Eigenvector** of covariance matrix, and **coefficients** of 2nd principal component

...

$\{a_{k1},a_{k2},...,a_{kk}\}$ is *k*th **Eigenvector** of covariance matrix, and **coefficients** of *k*th principal component

Computation of PCA

- The direction is given by the eigenvector γ_1 correponding to the largest eigenvalue of covariance matrix **C**
- The second vector that is orthogonal (uncorrelated) to the first is the one that has the second highest variance which comes to be the eignevector corresponding to the second eigenvalue
- And so on …



Calculating eigenvalues and eigenvectors

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- The eigenvalues λ_i are found by solving the equation

  $Cx = \lambda x$

  $det(C-\lambda I)=0$

- Eigenvectors are columns of the matrix *A* such that

  $C=A\ D\ A^T$

  where D is a diagonal matrix

$$D = \begin{pmatrix} \lambda_1 & 0 & \ldots\ldots & 0 \\ 0 & \lambda_2 & \ldots\ldots & 0 \\ 0 & & & \\ 0 & \ldots\ldots\ldots & \ldots & \lambda_p \end{pmatrix}$$

- In practice, the eigenvectors are computed by SVD (singular value decomposition).

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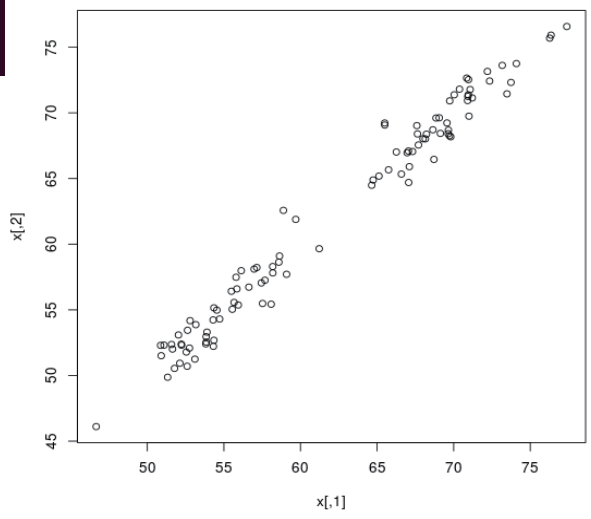
```
> X <- matrix(rnorm(32000), 1000, 32)
> dim(X)
[1] 1000   32
> pca_X <- prcomp(X)
> pca_X
Standard deviations (1, .., p=32):
 [1] 1.1611268 1.1515482 1.1477628 1.1316116 1.1165251 1.1021387 1.0869687
 [8] 1.0770949 1.0669926 1.0638087 1.0539471 1.0525123 1.0368192 1.0296589
[15] 1.0204239 1.0106765 1.0014669 0.9868647 0.9819980 0.9618256 0.9587249
[22] 0.9491361 0.9463531 0.9391354 0.9229802 0.9129457 0.9069524 0.8888694
[29] 0.8832288 0.8669869 0.8599976 0.8498946

Rotation (n x k) = (32 x 32):
              PC1          PC2         PC3          PC4          PC5
 [1,]  0.1273681775 -0.141384568  0.10253371 -0.025551064  0.063805435
 [2,] -0.0586362373 -0.097460978 -0.23289460  0.033280613 -0.057664530
 [3,] -0.0568348643 -0.145480526 -0.03000443 -0.364971502 -0.165182630
 [4,] -0.0267425081  0.217378536 -0.16041250  0.014201023 -0.256952950
 [5,] -0.4712193258 -0.166847283 -0.09229190 -0.059443440 -0.046960081
 [6,] -0.1614406885 -0.166437088 -0.21686270  0.168164903 -0.242285265
 [7,] -0.0014116763 -0.191471560  0.03982241 -0.050303873 -0.003665553
 [8,]  0.1099764928  0.400860439 -0.38249763  0.024063732  0.068599711
```

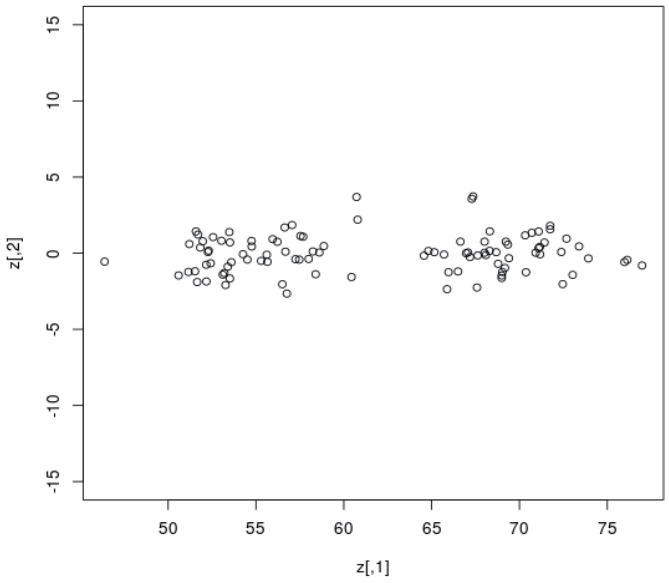
```
> summary(pca_X)
Importance of components:
                          PC1     PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     1.16113 1.15155 1.14776 1.13161 1.11653 1.10214 1.08697
Proportion of Variance 0.04146 0.04078 0.04051 0.03938 0.03834 0.03736 0.03633
Cumulative Proportion  0.04146 0.08224 0.12275 0.16213 0.20047 0.23783 0.27416
                          PC8     PC9    PC10    PC11    PC12    PC13    PC14
Standard deviation     1.07709 1.06699 1.0638 1.05395 1.05251 1.03682 1.0297
Proportion of Variance 0.03568 0.03501 0.0348 0.03416 0.03407 0.03306 0.0326
Cumulative Proportion  0.30984 0.34485 0.3796 0.41381 0.44788 0.48094 0.5135
                         PC15    PC16    PC17    PC18    PC19    PC20    PC21
Standard deviation     1.02042 1.01068 1.00147 0.98686 0.98200 0.96183 0.95872
Proportion of Variance 0.03202 0.03141 0.03084 0.02995 0.02966 0.02845 0.02827
Cumulative Proportion  0.54557 0.57698 0.60782 0.63777 0.66743 0.69588 0.72414
                          PC22    PC23    PC24   PC25    PC26   PC27   PC28
Standard deviation     0.9491 0.94635 0.93914 0.9230 0.91295 0.9070 0.8889
Proportion of Variance 0.0277 0.02754 0.02712 0.0262 0.02563 0.0253 0.0243
Cumulative Proportion  0.7519 0.77939 0.80651 0.8327 0.85834 0.8836 0.9079
                          PC29    PC30    PC31    PC32
Standard deviation     0.88323 0.86699 0.86000 0.84989
Proportion of Variance 0.02399 0.02312 0.02274 0.02221
Cumulative Proportion  0.93193 0.95504 0.97779 1.00000
> 
```



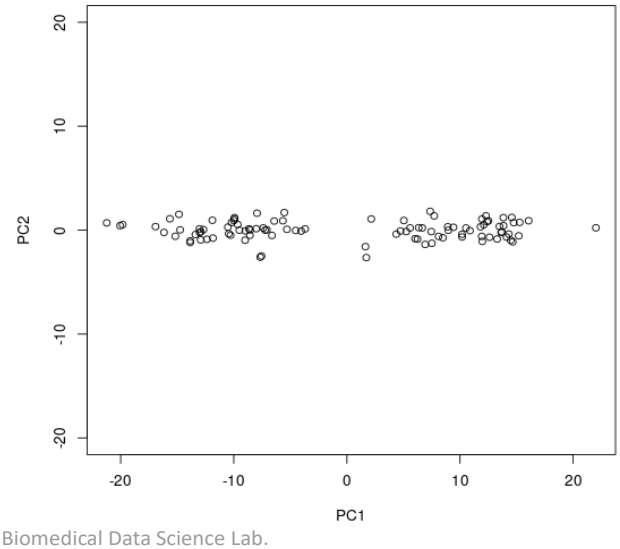
```
> set.seed(1988)
> library(MASS)
> n <- 100
> Sigma <- matrix(c(9, 9 * 0.9, 9 * 0.92, 9 * 1), 2, 2)
> x <- rbind(mvrnorm(n / 2, c(69, 69), Sigma),
+            mvrnorm(n / 2, c(55, 55), Sigma))
>
> dim(x)
[1] 100   2
```



```
> z  <- cbind((x[,2] + x[,1])/2,  x[,2] - x[,1])
```




```
> summary(prcomp(x))
Importance of components:
                          PC1     PC2
Standard deviation     11.357 0.88114
Proportion of Variance  0.994 0.00598
Cumulative Proportion   0.994 1.00000
```



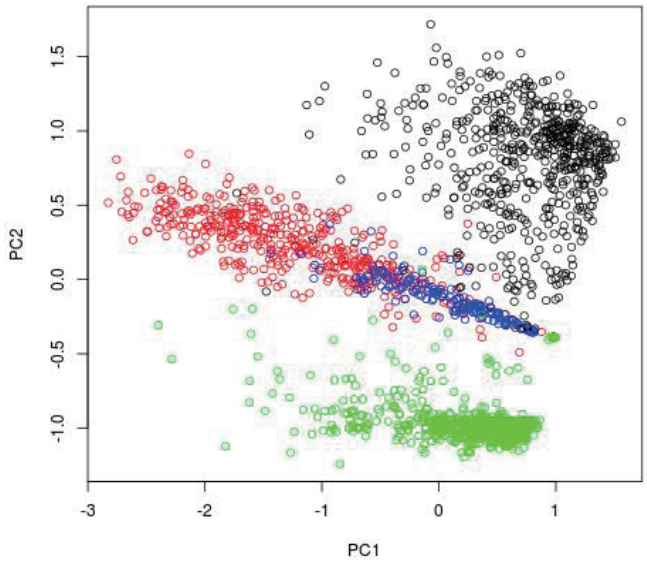
```
> head(USArrests)
           Murder Assault UrbanPop Rape
Alabama      13.2     236       58 21.2
Alaska       10.0     263       48 44.5
Arizona       8.1     294       80 31.0
Arkansas      8.8     190       50 19.5
California    9.0     276       91 40.6
Colorado      7.9     204       78 38.7
>
> pca_usarrests <- prcomp(USArrests)
> summary(pca_usarrests)
Importance of components:
                          PC1      PC2    PC3     PC4
Standard deviation     83.7324 14.21240 6.4894 2.48279
Proportion of Variance  0.9655  0.02782 0.0058 0.00085
Cumulative Proportion   0.9655  0.99335 0.9991 1.00000
>
> pca_usarrests$rotation
                PC1         PC2         PC3         PC4
Murder   0.04170432 -0.04482166  0.07989066 -0.99492173
Assault  0.99522128 -0.05876003 -0.06756974  0.03893830
UrbanPop 0.04633575  0.97685748 -0.20054629 -0.05816914
Rape     0.07515550  0.20071807  0.97408059  0.07232502
```


sklearn.decomposition.PCA

class sklearn.decomposition. **PCA**(*n_components=None, *, copy=True, whiten=False, svd_solver='auto', tol=0.0, iterated_power='auto', random_state=None*) [source]

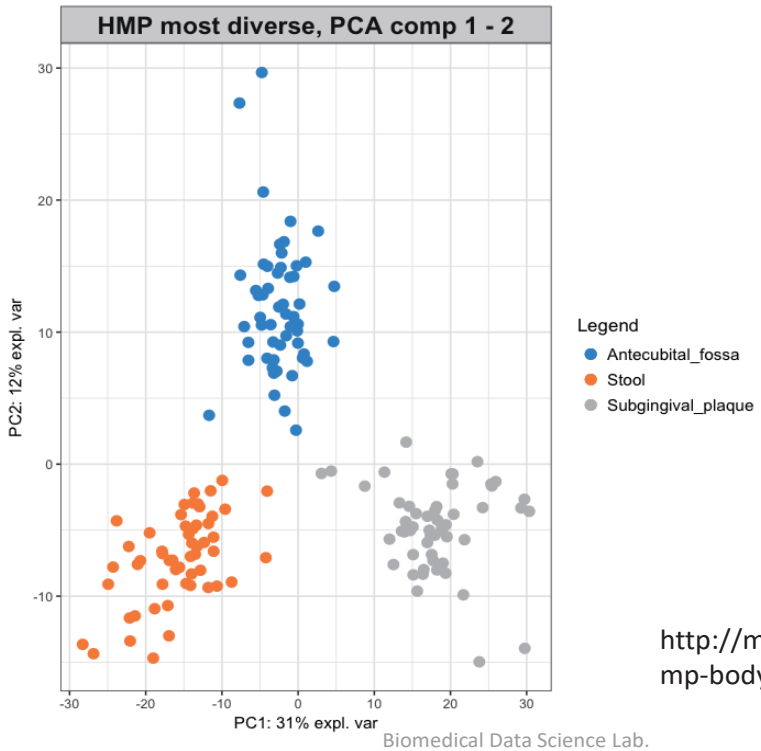
https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

PCA example for TCGA expression data



Red: COADREAD
Blue: GBM
Black: HNSC
Green: PRAD

PCA example for microbiome RNAseq



http://mixomics.org/mixmc/case-study-hmp-bodysites-repeated-measures/

Independent Component Analysis (ICA)

ICA

- Independent component analysis (ICA) is a method for finding underlying factors or components from multivariate (multi-dimensional) statistical data.
- It looks for components that are both *statistically independent*, and *nonGaussian*.

- The two broadest definitions of independence for ICA are

  1) Minimization of Mutual Information
  2) Maximization of non-Gaussianity

ICA

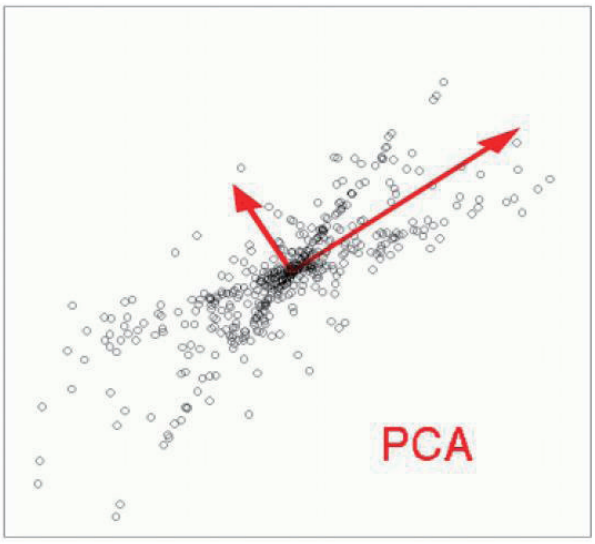
- For example, given two-dimensional vector , $\boldsymbol{x} = [\, x_1\, x_2\,]^T$, ICA aims at finding the following decomposition

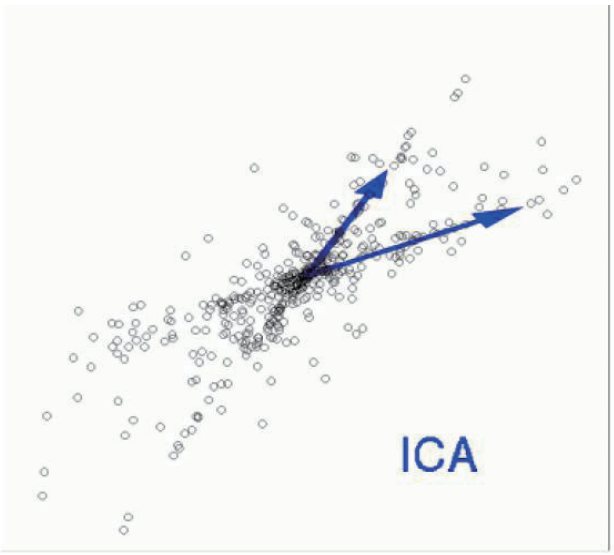
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix} s_1 + \begin{bmatrix} a_{12} \\ a_{22} \end{bmatrix} s_2$$

$$\boldsymbol{x} = \boldsymbol{a}_1 s_1 + \boldsymbol{a}_2 s_2$$

where $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ are basis vectors and s_1, s_2 are basis coefficients.

- Constraint: Basis coefficients s_1 and s_2 are statistically independent





sklearn.decomposition.FastICA

class `sklearn.decomposition.` **`FastICA`**(*n_components=None, *, algorithm='parallel', whiten=True, fun='logcosh', fun_args=None, max_iter=200, tol=0.0001, w_init=None, random_state=None*) [source]

FastICA: a fast algorithm for Independent Component Analysis.

https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.FastICA.html

Non-negative Matrix Factorization (NMF)

nature
International journal of science

Letter | Published: 21 October 1999

Learning the parts of objects by non-negative matrix factorization

Daniel D. Lee & H. Sebastian Seung

Nature **401**, 788–791 (1999) | Download Citation

Algorithms for Non-negative Matrix Factorization

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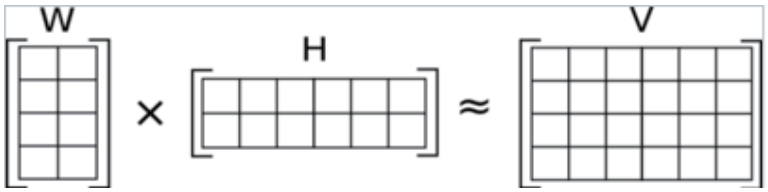
*Bell Laboratories
Lucent Technologies
Murray Hill, NJ 07974

H. Sebastian Seung*†
†Dept. of Brain and Cog. Sci.
Massachusetts Institute of Technology
Cambridge, MA 02138

NMF



From Wikipedia

- **Non-negative matrix factorization** (**NMF** or **NNMF**), also **non-negative matrix approximation** is a group of algorithms in multivariate analysis a nd linear algebra where a matrix **V** is factorized into (usually) two matric es **W** and **H**, with the property that all three matrices have no negative e lements.
- The matrix **V** is represented by the two smaller matrices **W** and **H**, which , when multiplied, approximately reconstruct **V**.

PNAS Proceedings of the National Academy of Sciences of the United States of America

Keyword

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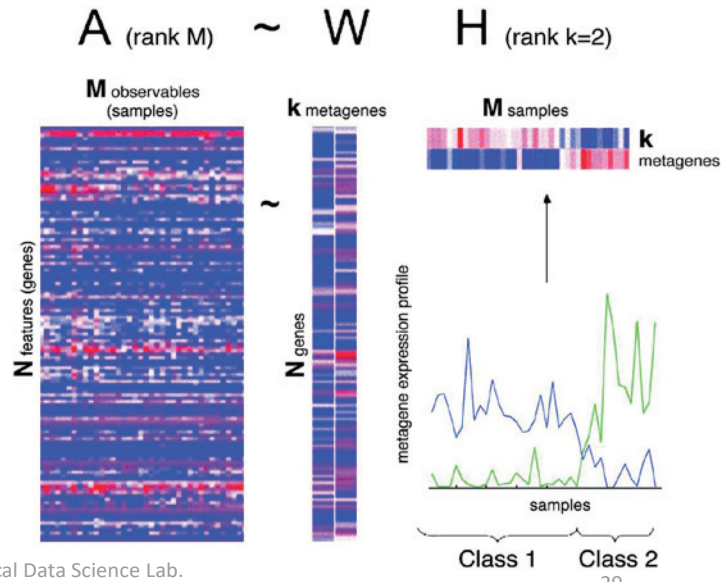
NEW RESEARCH IN Physical Sciences | Social Sciences

Metagenes and molecular pattern discovery using matrix factorization

Jean-Philippe Brunet, Pablo Tamayo, Todd R. Golub, and Jill P. Mesirov

PNAS March 23, 2004 101 (12) 4164-4169; https://doi.org/10.1073/pnas.0308531101



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Archive > Volume 500 > Issue 7463 > Articles > Article

NATURE | ARTICLE

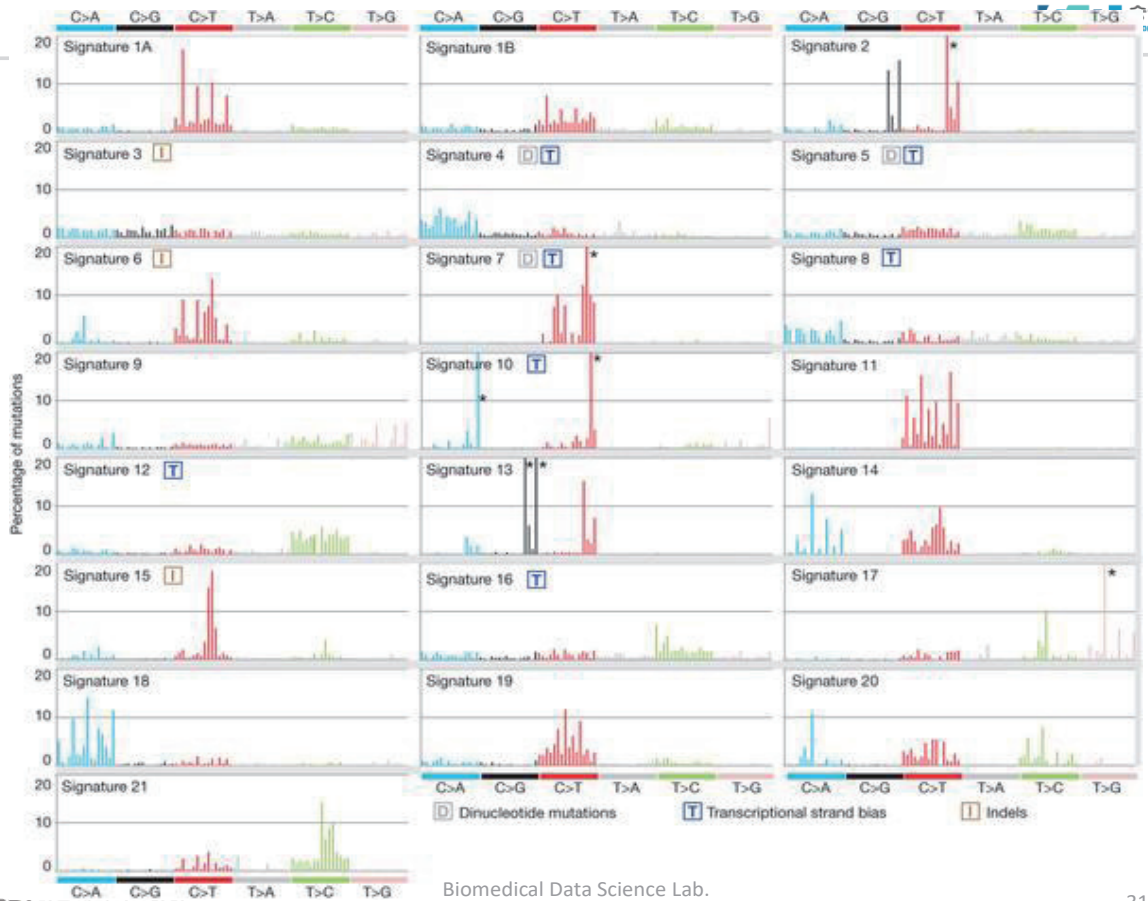
日本語要約

Signatures of mutational processes in human cancer

Ludmil B. Alexandrov, Serena Nik-Zainal, David C. Wedge, Samuel A. J. R. Aparicio, Sam Behjati, Andrew V. Biankin, Graham R. Bignell, Niccolò Bolli, Ake Borg, Anne-Lise Børresen-Dale, Sandrine Boyault, Birgit Burkhardt, Adam P. Butler, Carlos Caldas, Helen R. Davies, Christine Desmedt, Roland Eils, Jórunn Erla Eyfjörd, John A. Foekens, Mel Greaves, Fumie Hosoda, Barbara Hutter, Tomislav Ilicic, Sandrine Imbeaud, Marcin Imielinsk + et al.

Affiliations | Contributions | Corresponding author

Nature 500, 415–421 (22 August 2013) | doi:10.1038/nature12477
Received 24 March 2013 | Accepted 19 July 2013 | Published online 14 August 2013



COSMIC
Catalogue of somatic mutations in cancer

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- Whole Genomes
- Cell Lines Project
- COSMIC
- Cancer Gene Census
- Drug Sensitivity
- Mutational Signatures
- GRCh37 Archive

Signatur…s in Human Cancer

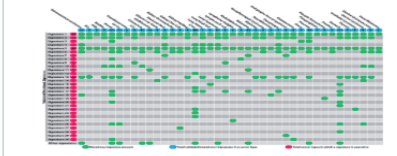
Somatic m…lls of the human body and occur throughout life. They are the consequence of multip…luding the intrinsic slight infidelity of the DNA replication machinery, exogenou…posures, enzymatic modification of DNA and defective DNA repair. Different mutationa…combinations of mutation types, termed "Mutational Signatures".

In the pas… have revealed many mutational signatures across the spectrum of human cancer types [Nik… …exandrov L.B. *et al.*, Cell Reports (2013); Alexandrov L.B. *et al.*, Nature (2013); Helleday T… …Alexandrov L.B. and Stratton M.R., Curr Opin Genet Dev (2014)]. However, as the number of … …need for a curated census of signatures has become apparent. Here, we deliver such a resource … …additional information about, known mutational signatures.

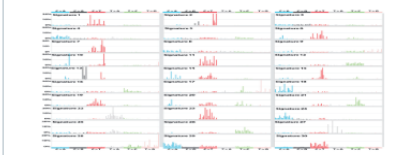
The curr… …d on an analysis of 10,952 exomes and 1,048 whole-genomes across 40 distinct types of hu… …based on curated data that were generated by The Cancer Genome Atlas (TCGA), the Inte… …um (ICGC), and a large set of freely available somatic mutations published in peer-reviewe… …ata sources will be provided in future releases of COSMIC.

The profile… …using the six substitution subtypes: C>A, C>G, C>T, T>A, T>C, and T>G (all substitution… …dine of the mutated Watson–Crick base pair). Further, each of the substitutions is examined by incorporating information on the bases immediately 5′ and 3′ to each mutated base generating 96 possible mutation types (6 types of substitution • 4 types of 5′ base • 4 types of 3′ base). Mutational signatures are displayed and reported based on the observed trinucleotide frequency of the human genome, i.e., representing the relative proportions of mutations generated by each signature based on the actual trinucleotide frequencies of the reference human genome version GRCh37. Note that only validated mutational signatures have been included in the curated census of mutational signatures.

Additional information is provided for each signature, including the cancer types in which the signature has been found, proposed aetiology for the mutational processes underlying the signature, other mutational features that are associated with each signature and information that may be relevant for better understanding of a particular mutational signature.



Mutational signatures across human cancer



Patterns of mutational signatures [Download signatures]

```
# Install
install.packages('NMF')
# Load
library(NMF)
```



```
mat <- matrix(runif(n= 200, min= 0, max=
100), nrow= 30, ncol= 10)

res<- nmf(mat, rank= 2)
w<- basis(res)
h<- coef(res)

w %*% h # ~ mat
dim(w) # 30 2
```

sklearn.decomposition.NMF

class `sklearn.decomposition.` **`NMF`**(*n_components=None, *, init='warn', solver='cd', beta_loss='frobenius', tol=0.0001, max_iter=200, random_state=None, alpha=0.0, l1_ratio=0.0, verbose=0, shuffle=False, regularization='both'*) [source]

Non-Negative Matrix Factorization (NMF).

Examples

```
>>> import numpy as np
>>> X = np.array([[1, 1], [2, 1], [3, 1.2], [4, 1], [5, 0.8], [6, 1]])
>>> from sklearn.decomposition import NMF
>>> model = NMF(n_components=2, init='random', random_state=0)
>>> W = model.fit_transform(X)
>>> H = model.components_
```

Methods

`fit`(X[, y])	Learn a NMF model for the data X.
`fit_transform`(X[, y, W, H])	Learn a NMF model for the data X and returns the transformed data.
`get_params`([deep])	Get parameters for this estimator.
`inverse_transform`(W)	Transform data back to its original space.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X)	Transform the data X according to the fitted NMF model.

https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.NMF.html

t-SNE

t-distributed Stochastic Neighbor Embedding (t-SNE)

- T-distributed Stochastic Neighbor Embedding (t-SNE) is a ma chine learning algorithm for visualization developed by Laur ens van der Maaten and Geoffrey Hinton.
- It is a nonlinear dimensionality reduction technique well-sui ted for embedding high-dimensional data for visualization in a low-dimensional space of two or three dimensions.

```
> install.packages("Rtsne")
```

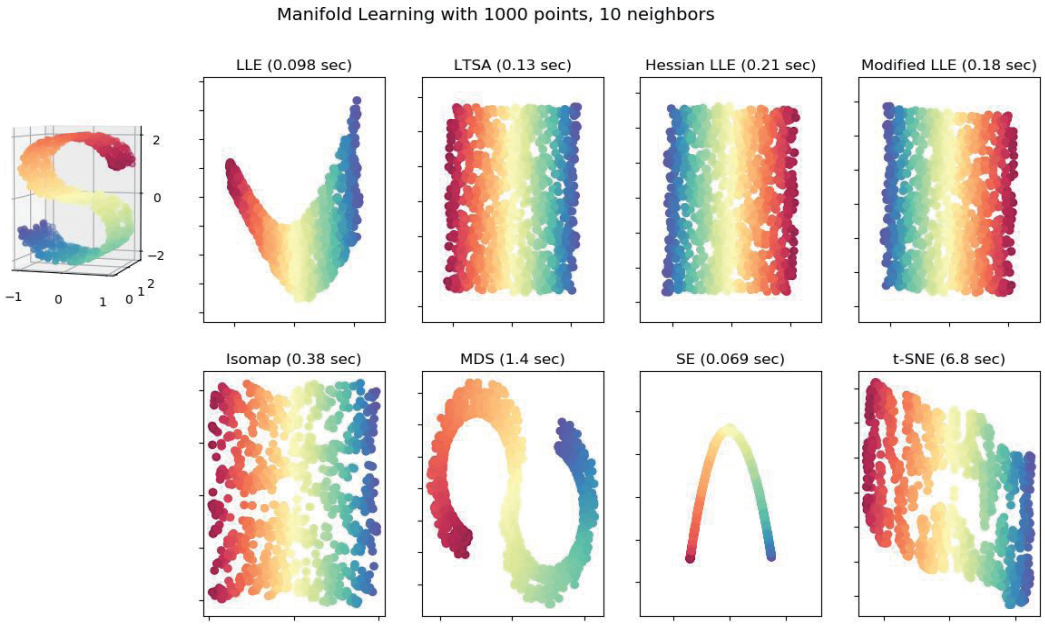

sklearn.manifold.TSNE

class sklearn.manifold.**TSNE**(*n_components=2*, ***, *perplexity=30.0*, *early_exaggeration=12.0*, *learning_rate=200.0*, *n_iter=1000*, *n_iter_without_progress=300*, *min_grad_norm=1e-07*, *metric='euclidean'*, *init='random'*, *verbose=0*, *random_state=None*, *method='barnes_hut'*, *angle=0.5*, *n_jobs=None*, *square_distances='legacy'*) [source]

t-distributed Stochastic Neighbor Embedding.

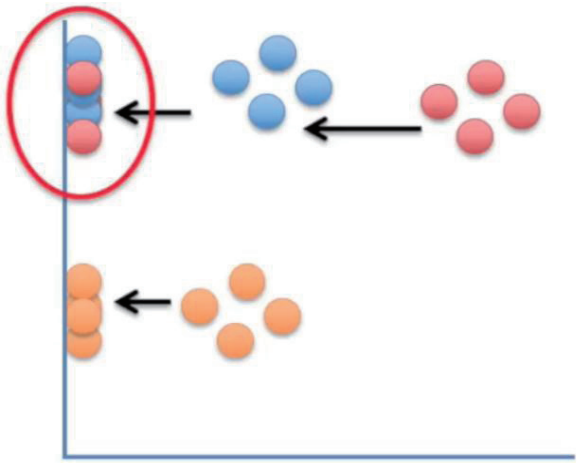
https://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html

Manifold learning

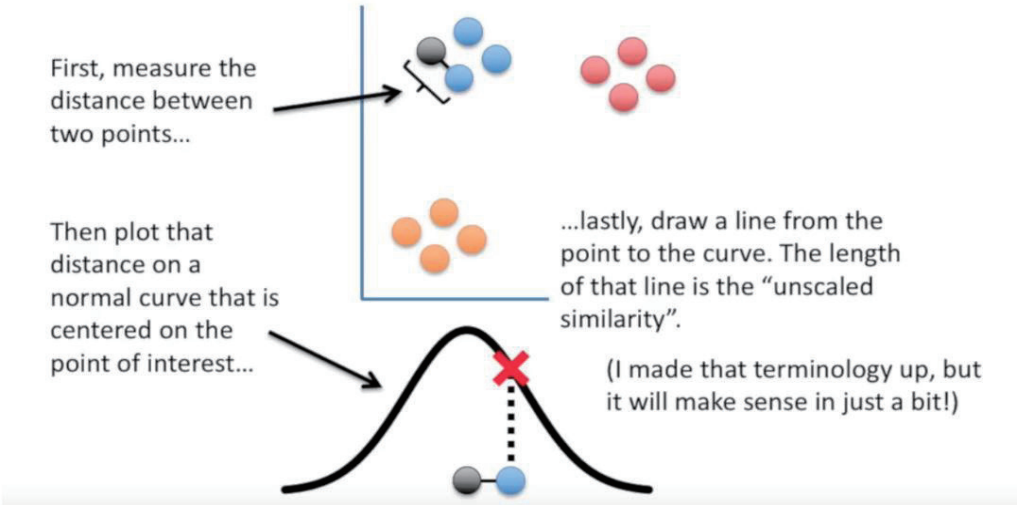


https://scikit-learn.org/stable/modules/manifold.html

PCA



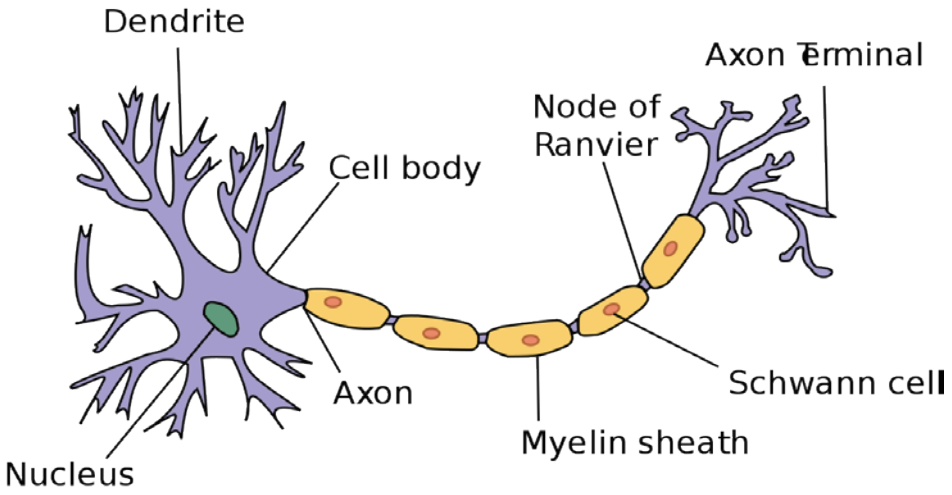
https://www.youtube.com/watch?v=NEaUSP4YerM



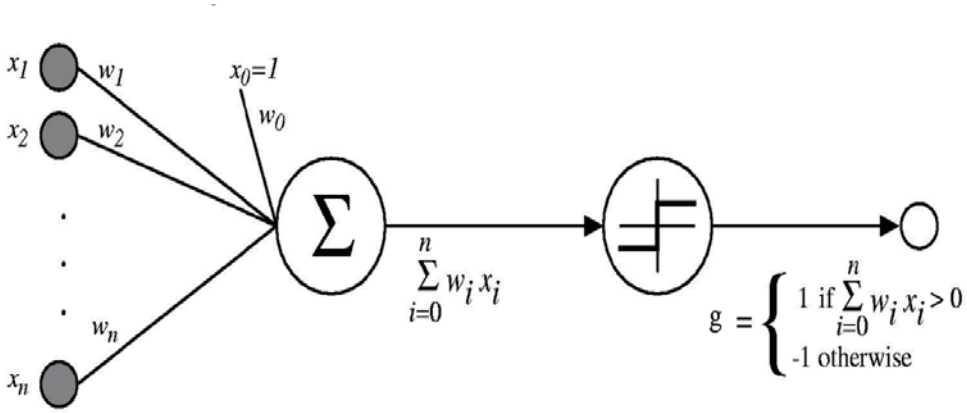
https://www.youtube.com/watch?v=NEaUSP4YerM

Deep Learning & Autoencoder

Human neuron



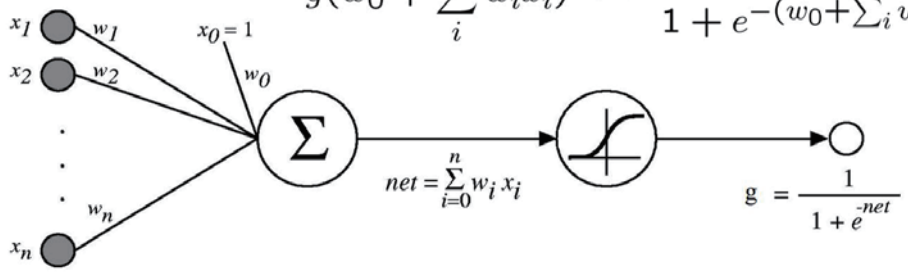
Perceptron as a neuron



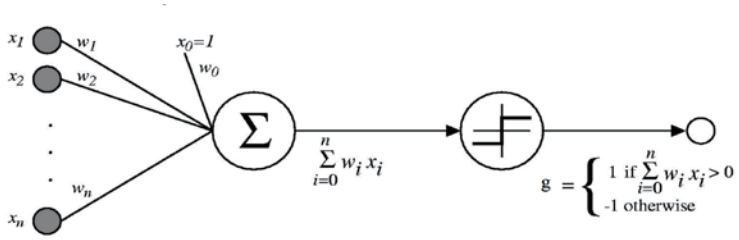
- $x_1, x_2, \ldots, x_n$ as inputs
- Sum is passed through **activation function** g()

Sigmoid neuron

$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$



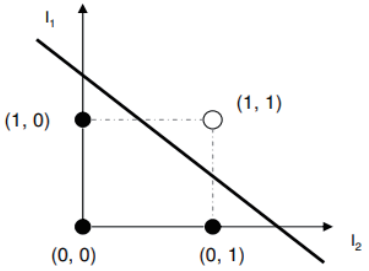
XOR problem



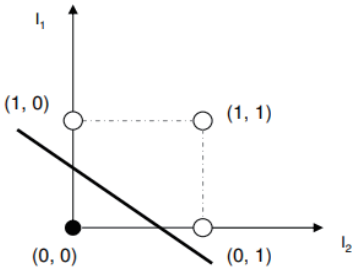
XOR truth table

Input		Output
A	B	
0	0	0
0	1	1
1	0	1
1	1	0

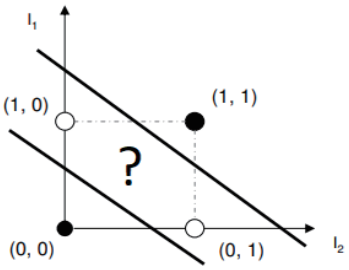
AND		
I_1	I_2	out
0	0	0
0	1	0
1	0	0
1	1	1



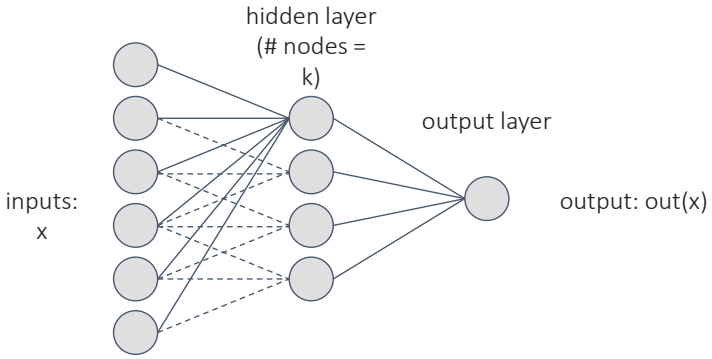
OR		
I_1	I_2	out
0	0	0
0	1	1
1	0	1
1	1	1



XOR		
I_1	I_2	out
0	0	0
0	1	1
1	0	1
1	1	0



Multilayer percepton



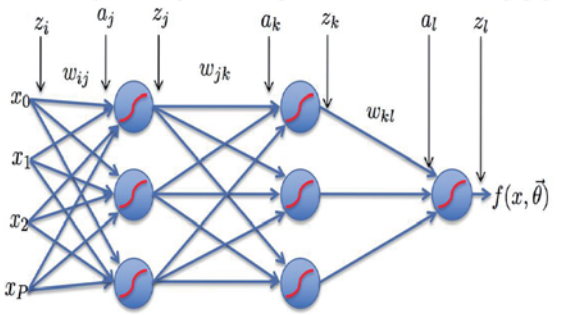
$$out(x) = g(w_0 + \Sigma w_k g(\Sigma w_i^k x_i))$$

Backpropagation of errors

$$R(\theta) = \frac{1}{N}\sum_{n=0}^{N} L(y_n - f(x_n)) \quad \text{Empirical Risk Function}$$

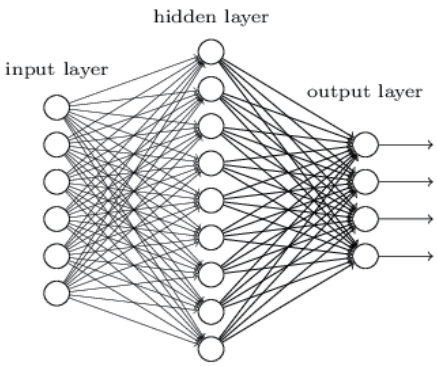
$$= \frac{1}{N}\sum_{n=0}^{N} \frac{1}{2}(y_n - f(x_n))^2$$

$$= \frac{1}{N}\sum_{n=0}^{N} \frac{1}{2}\left(y_n - g\left(\sum_k w_{kl} g\left(\sum_j w_{jk} g\left(\sum_i w_{ij} x_{n,i}\right)\right)\right)\right)^2$$

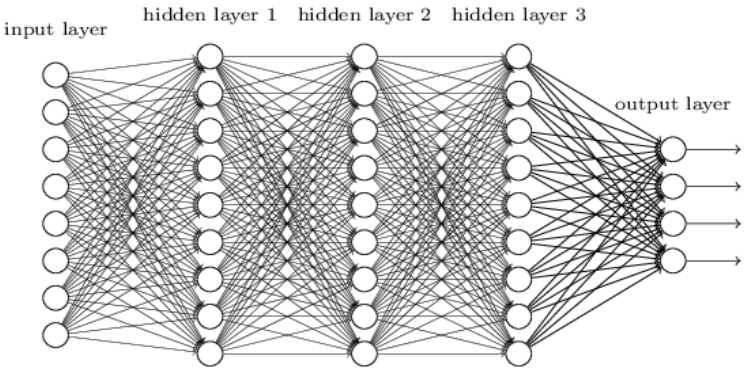


Deep neural networks

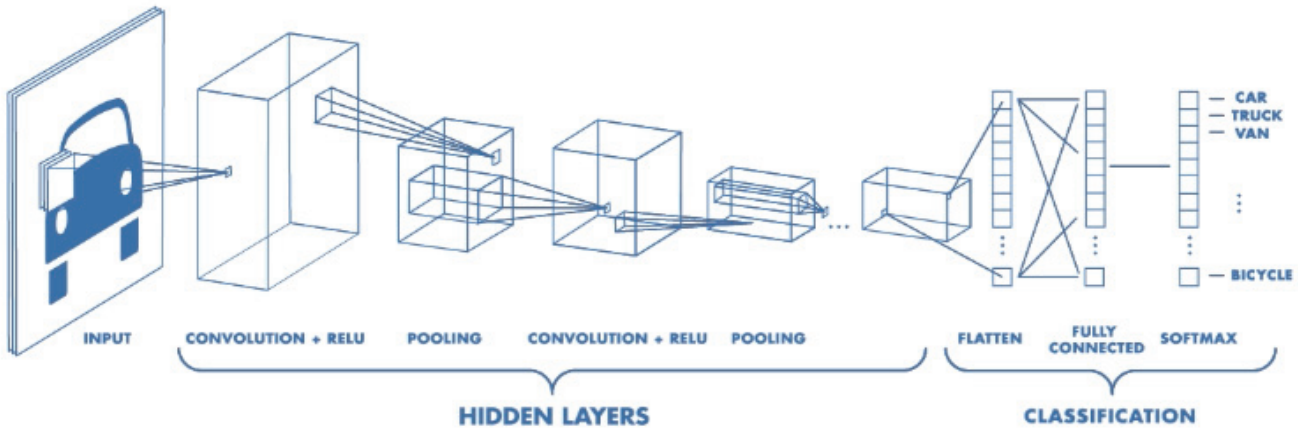
"Non-deep" feedforward neural network



Deep neural network

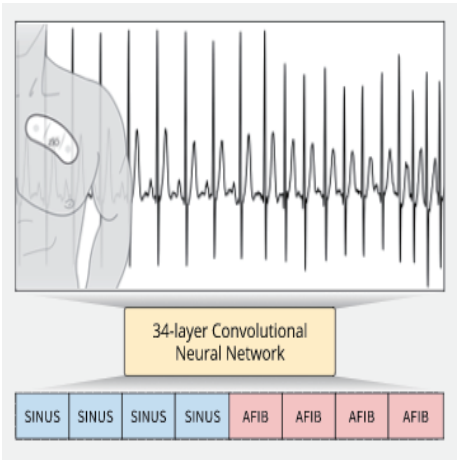


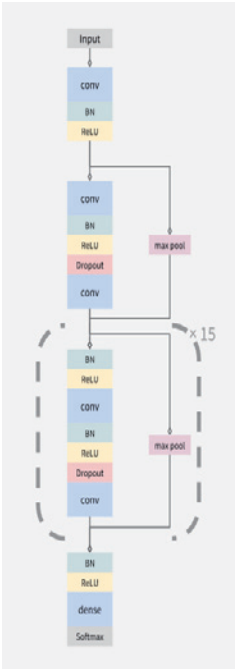
Convolutional Neural Networks



Cardiologist-Level Arrhythmia Detection With Convolutional Neural Networks

- They have a dataset of 64,121 ECG records from 29,163 patients.
- The model outperforms the cardiologist average on both the Sequence and Set F1 metrics

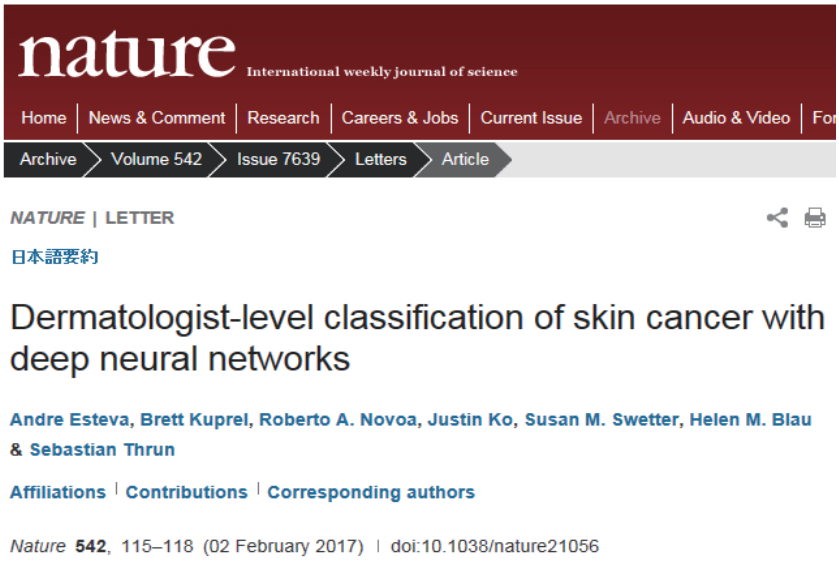




https://stanfordmlgroup.github.io/projects/ecg/

Skin Cancer Detection

숭실대학교 Soongsil University



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Archive > Volume 542 > Issue 7639 > Letters > Article

NATURE | LETTER

日本語要約

Dermatologist-level classification of skin cancer with deep neural networks

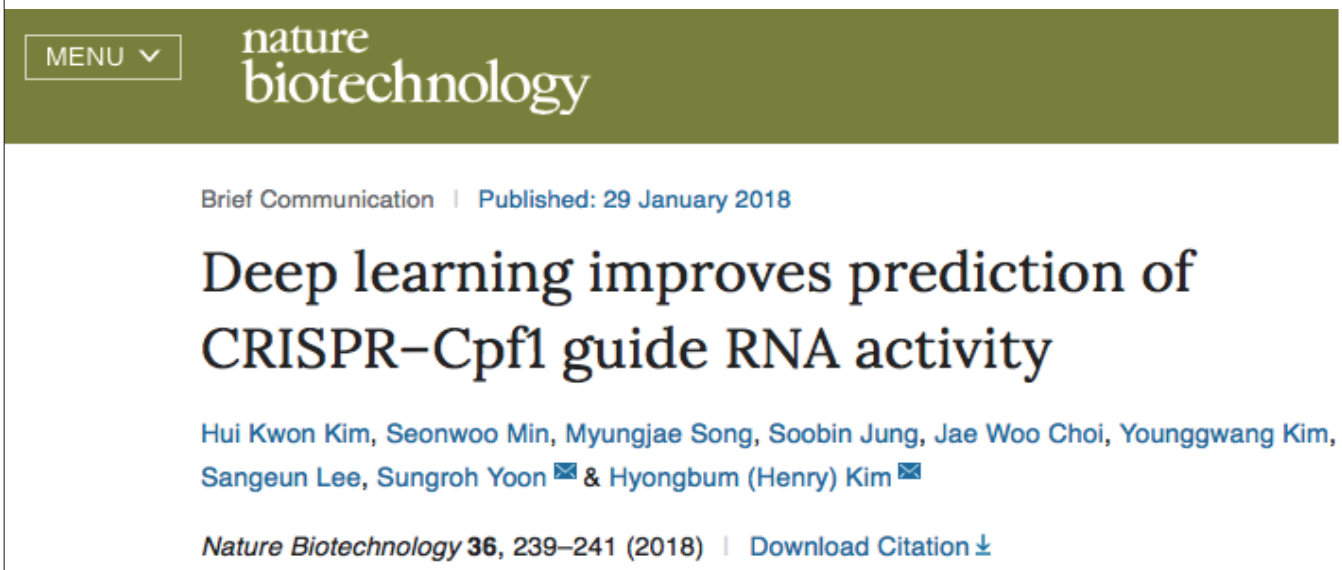
Andre Esteva, Brett Kuprel, Roberto A. Novoa, Justin Ko, Susan M. Swetter, Helen M. Blau & Sebastian Thrun

Affiliations | Contributions | Corresponding authors

Nature **542**, 115–118 (02 February 2017) | doi:10.1038/nature21056

- 5.4 million new cases of skin cancer in USA every year.
- Melanomas represent fewer than 5% but they account for 75% of all skin cancer deaths
- Early detection is critical (survival rate would be 99% at early stage, but 14% at latest stage)

숭실대학교 Soongsil University



MENU

nature biotechnology

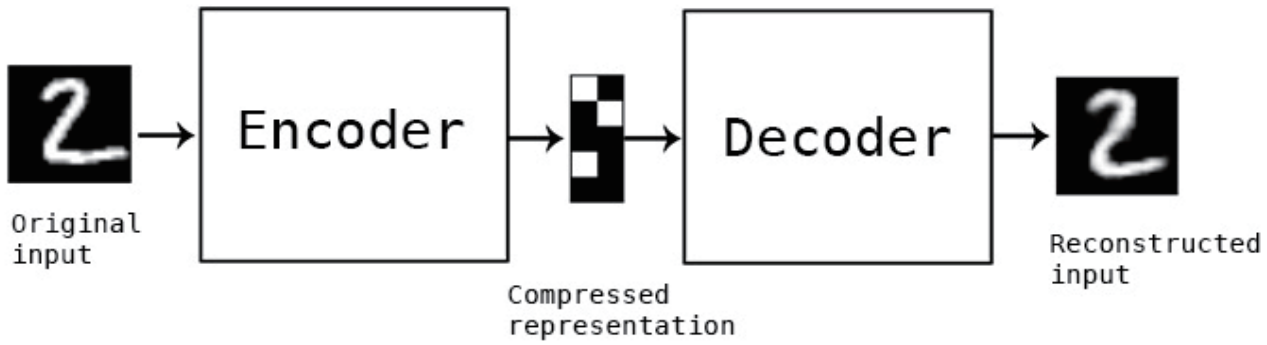
Brief Communication | Published: 29 January 2018

Deep learning improves prediction of CRISPR–Cpf1 guide RNA activity

Hui Kwon Kim, Seonwoo Min, Myungjae Song, Soobin Jung, Jae Woo Choi, Younggwang Kim, Sangeun Lee, Sungroh Yoon ✉ & Hyongbum (Henry) Kim ✉

Nature Biotechnology **36**, 239–241 (2018) | Download Citation ↓

Autoencoder



Keras example

```
from keras import layers

# This is the size of our encoded representations
encoding_dim = 32

# This is our input image
input_img = keras.Input(shape=(784,))

# "encoded" is the encoded representation of the input
encoded = layers.Dense(encoding_dim, activation='relu')(input_img)

# "decoded" is the lossy reconstruction of the input
decoded = layers.Dense(784, activation='sigmoid')(encoded)

# This model maps an input to its reconstruction
autoencoder = keras.Model(input_img, decoded)
```

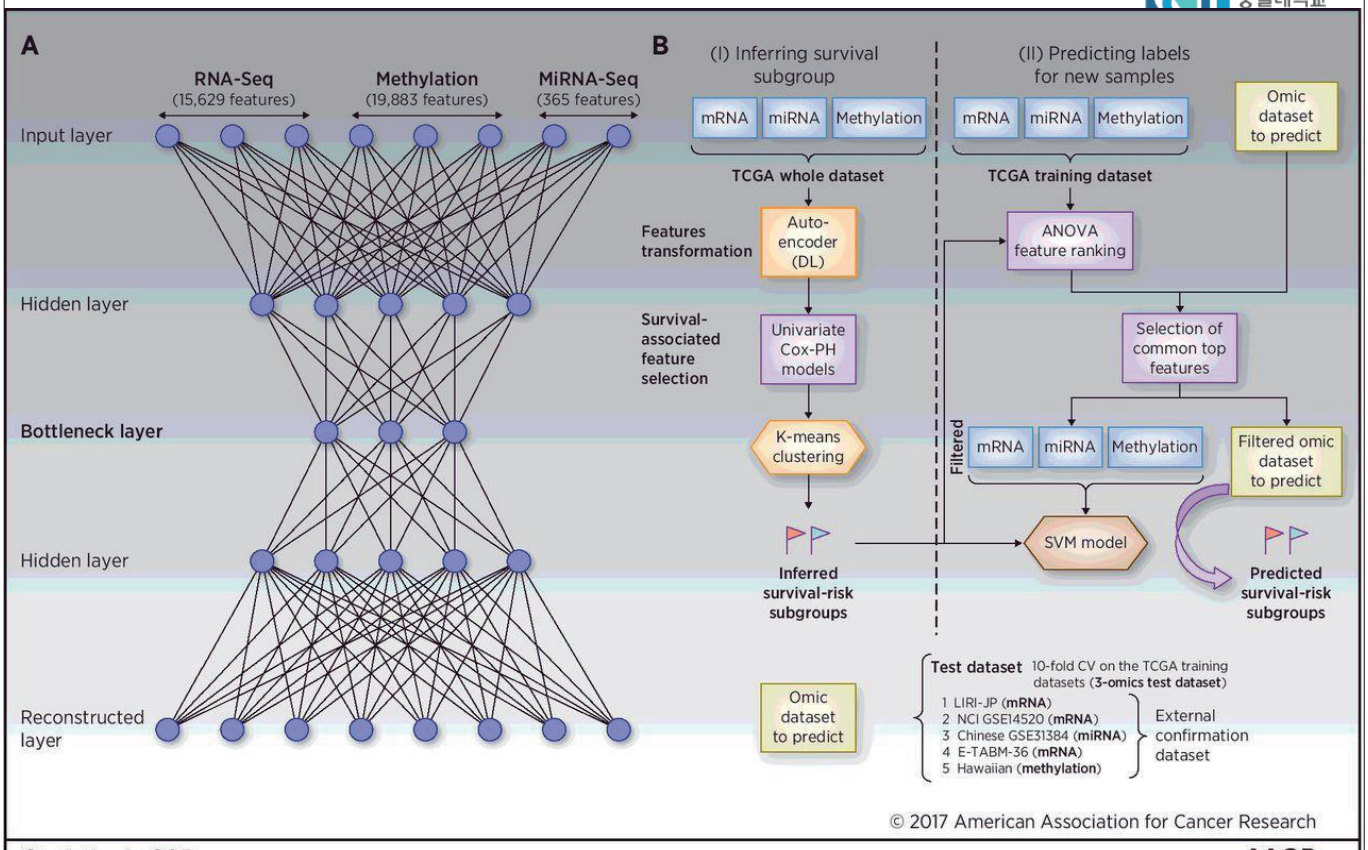
Deep autoencoder

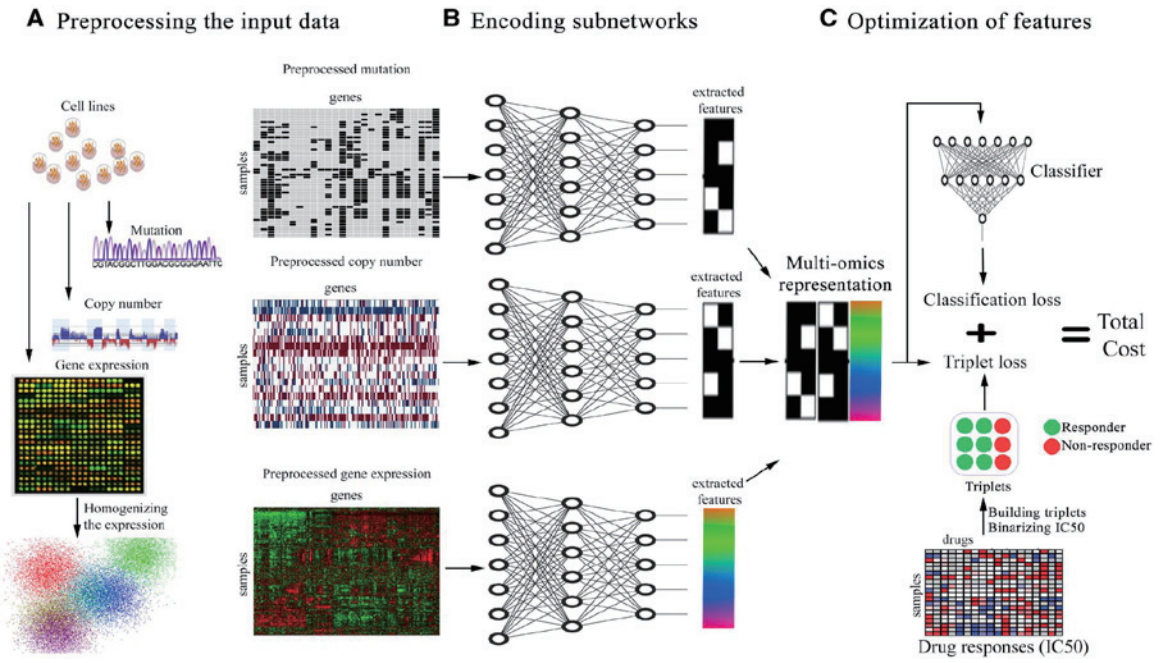
```
input_img = keras.Input(shape=(784,))
encoded = layers.Dense(128, activation='relu')(input_img)
encoded = layers.Dense(64, activation='relu')(encoded)
encoded = layers.Dense(32, activation='relu')(encoded)

decoded = layers.Dense(64, activation='relu')(encoded)
decoded = layers.Dense(128, activation='relu')(decoded)
decoded = layers.Dense(784, activation='sigmoid')(decoded)

autoencoder = keras.Model(input_img, decoded)
autoencoder.compile(optimizer='adam', loss='binary_crossentropy')

autoencoder.fit(x_train, x_train,
                epochs=100,
                batch_size=256,
                shuffle=True,
                validation_data=(x_test, x_test))
```

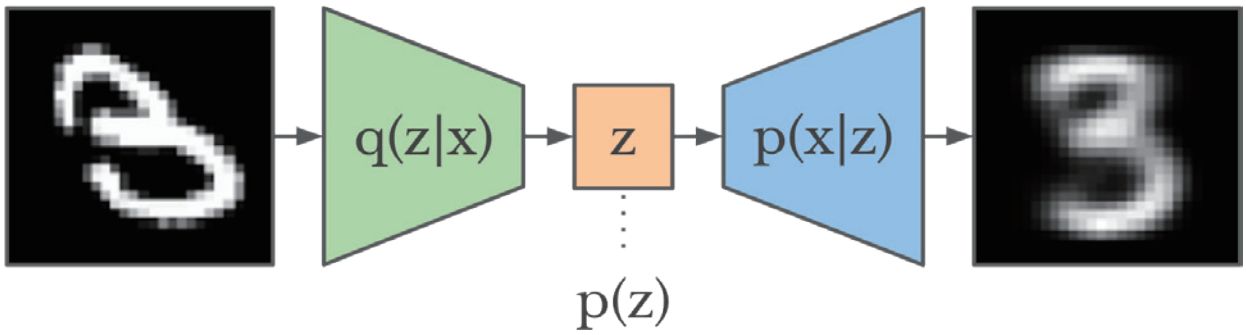





https://academic.oup.com/bioinformatics/article/35/14/i501/5529255

Variational Autoencoder

A VAE consist of three components: an encoder q(z|x), a prior p(z), and a decoder p(x|z).



https://danijar.com/building-variational-auto-encoders-in-tensorflow/

Variational Autoencoder

숭실대학교 Soongsil University

- Autoencoders learn a “compressed representation” of input (*could be image,text sequence etc.)* automatically by first co mpressing the input (*encoder*) and decompressing it back (*d ecoder*) to match the original input.

- Variational autoencoders learn the parameters of a probabili ty distribution representing the data. Since it learns to mode l the data, we can sample from the distribution and generat e new input data samples.

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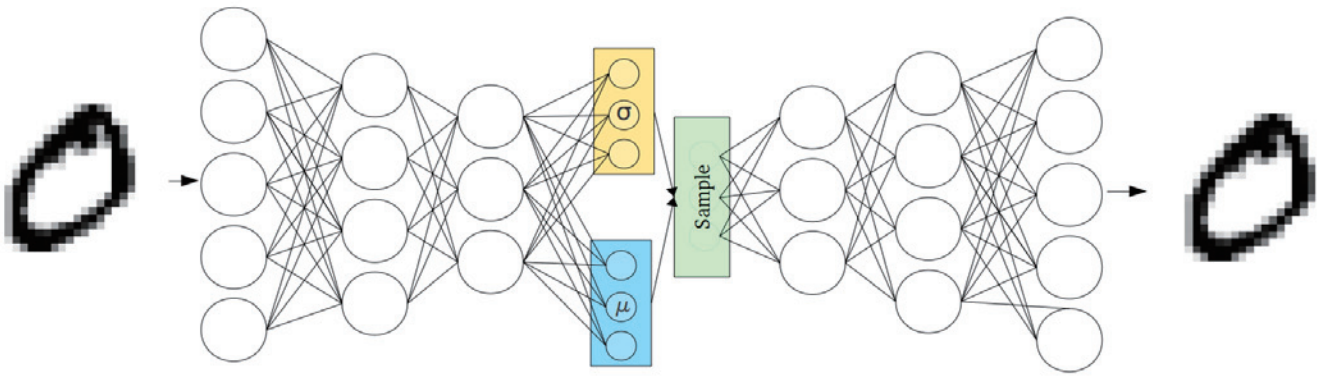
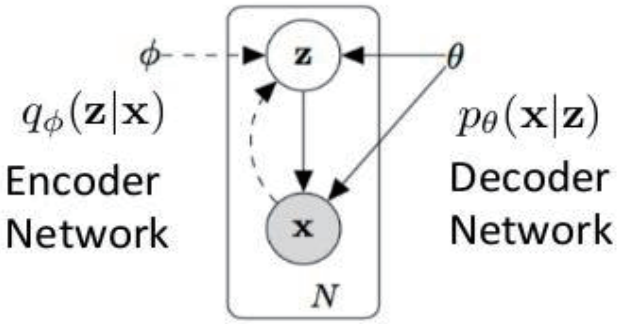


Variational autoencoder

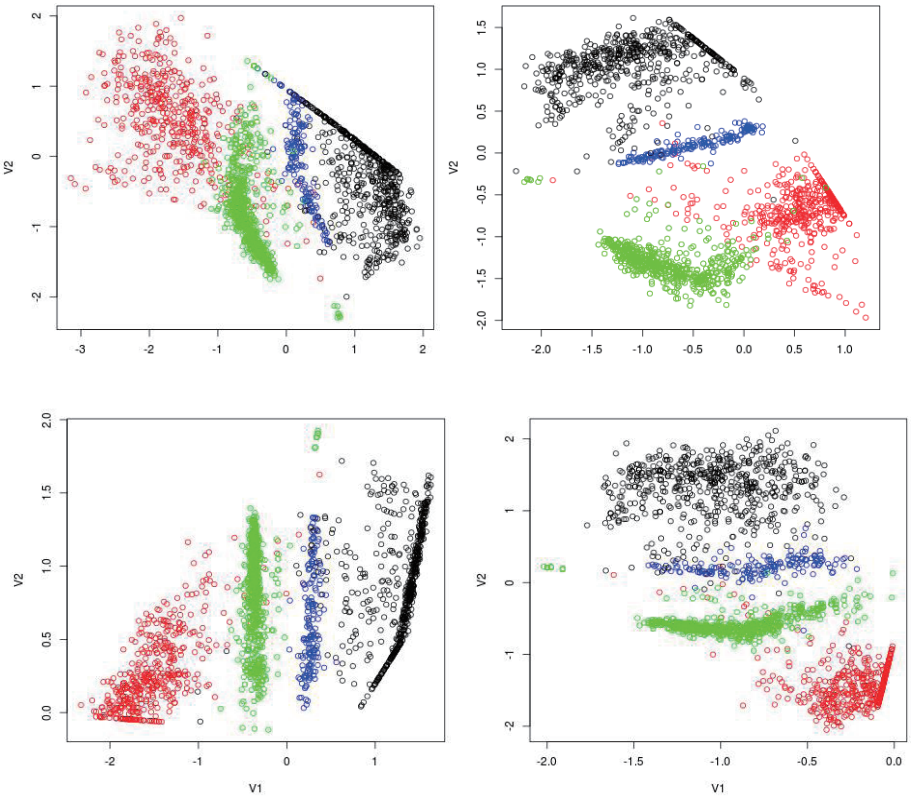


Minimize: $D_{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})]$

Intractable: $p_\theta(\mathbf{z}|\mathbf{x}) = \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{p_\theta(\mathbf{x})}$

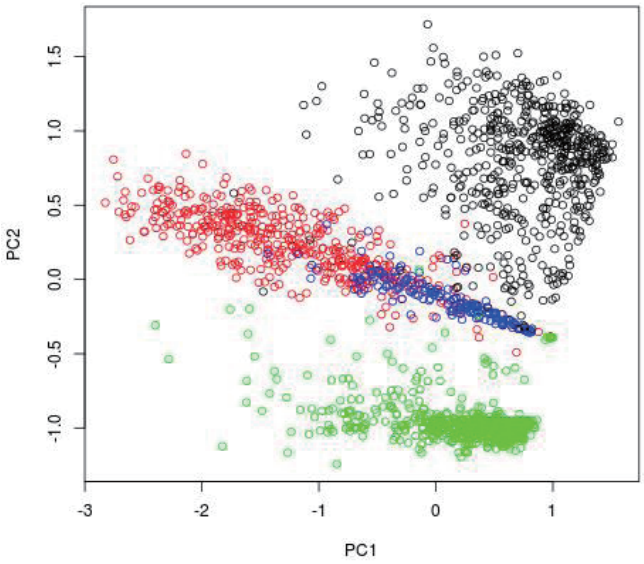
https://www.slideshare.net/ckmarkohchang/variational-autoencoder

VAE – TCGA expression



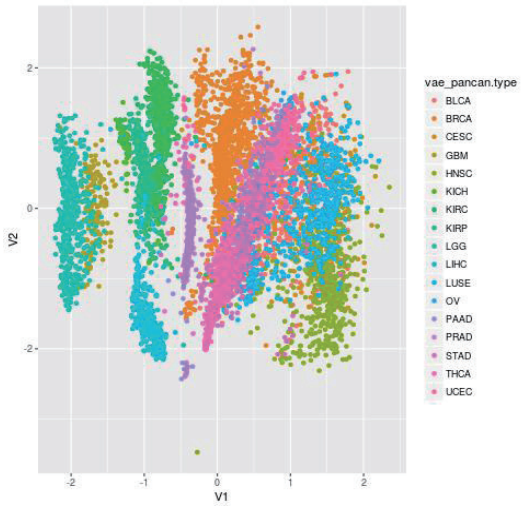
Red: COADREAD
Blue: GBM
Black: HNSC
Green: PRAD

PCA

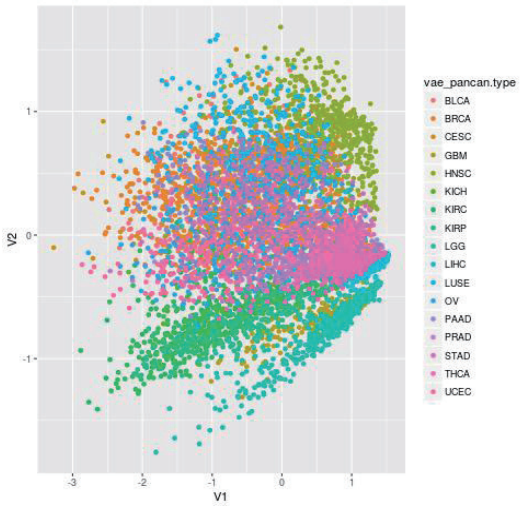


Red: COADREAD
Blue: GBM
Black: HNSC
Green: PRAD

VAE



PCA



Thank you