Data Science

2020/06/12 Course 3

Machine Learning II: PCA, regression, sequential data analysis, deep learning

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7. PCA・PLS (development of organic materials) and Pareto solutions (Catalyst design)

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7. PCAとPLS(有機材料の開発)、パレート最適解(触媒設計)

Preface

- **Environments for Data Science**
  - Editor

    Atom, Vim, Emacs
  - IDE

    Eclipse, Visual Studio, XCode, etc…
  - Interactive

    Jupyter (via Anaconda)
  - Cloud

    Google Colaboratory, MS Azure, AWS, Kaggle, etc…

Preface

- **Modeling and Learning**
  - Why we need models?
  - What is "learning" in data science?
  - How can we know which modeling is better?

Principal Component Analysis (PCA)
（主成分分析）

PCA

- **Principal Component Analysis**
  - Linear method to **reduce variable dimension.**
  - Pros

    Easy to apply, simple to interpret.
  - Cons

    Not suitable for noisy, high dimensional data.

  - Currently we have many other non-linear models for dimension reduction, though PCA is still useful for simple data.

PCA

- **Principal Components**
  - PC is a vector that maximize the variance of the given multidimensional variables.
  - Thus, the first PC is defined as below,

$$\mathbf{v_1} = \mathrm{argmax}_{|\mathbf{v}|=1} |X\mathbf{v}|^2$$

    where X is given variable set.

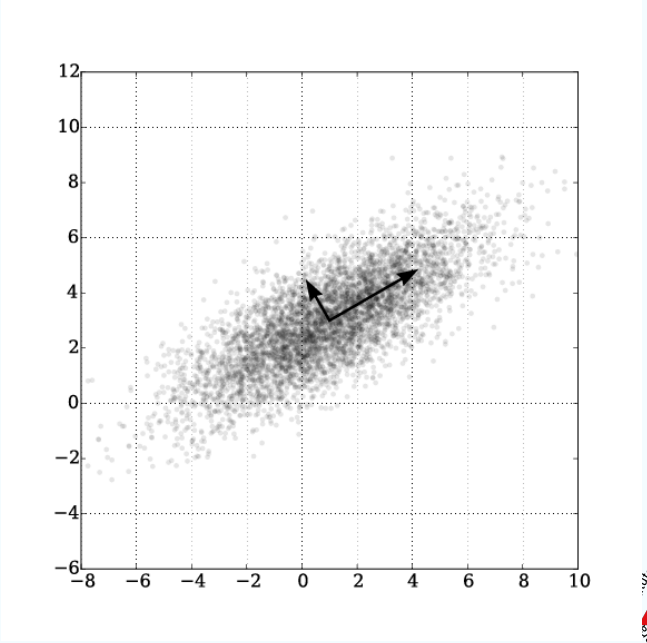
  - And subsequent components are,

$$X_{i+1} = X_i - X\mathbf{v}_i$$

$$\mathbf{v_i} = \mathrm{argmax}_{|\mathbf{v}|=1} |X_i\mathbf{v}|^2$$

PCA

- **Score**
  - Components of original variables X along with each PC.
- **Contribution**
  - Covariance of X with each PC divided by the total variance.
- **Rotation**
  - Transformation matrix from original to PC score.



PCA

- **Singular Value Decomposition (SVD)**
  - PCA can be regarded as one of the applications of singular value decomposition.

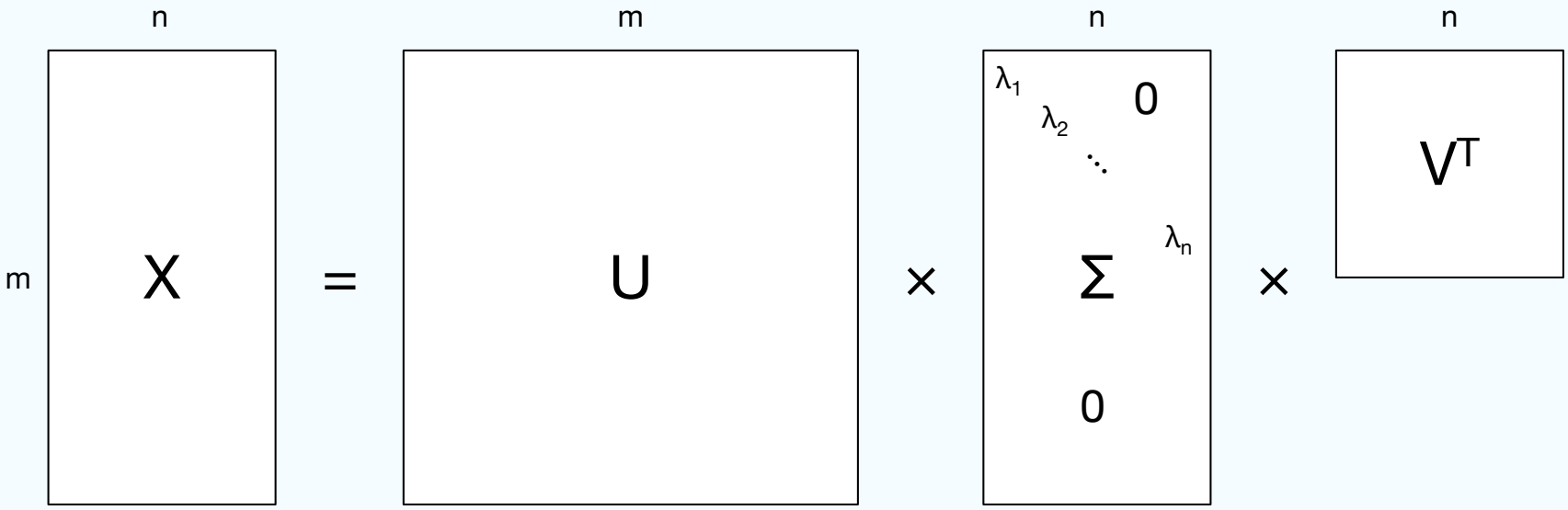
  - For any matrix X, there exists unitary matrixes U, V and Σ, which diagonal elements are non-negative and other elements are 0, that satisfies,

$$X = U\Sigma V^T$$

Unlike eigenvalue decomposition, X can be any $m \times n$ matrix.

PCA

- **Singular Value Decomposition (SVD)**



If $m < n$, Σ will be a horizontal matrix.

PCA

- For any matrix X there exists U, V and Σ, such that,

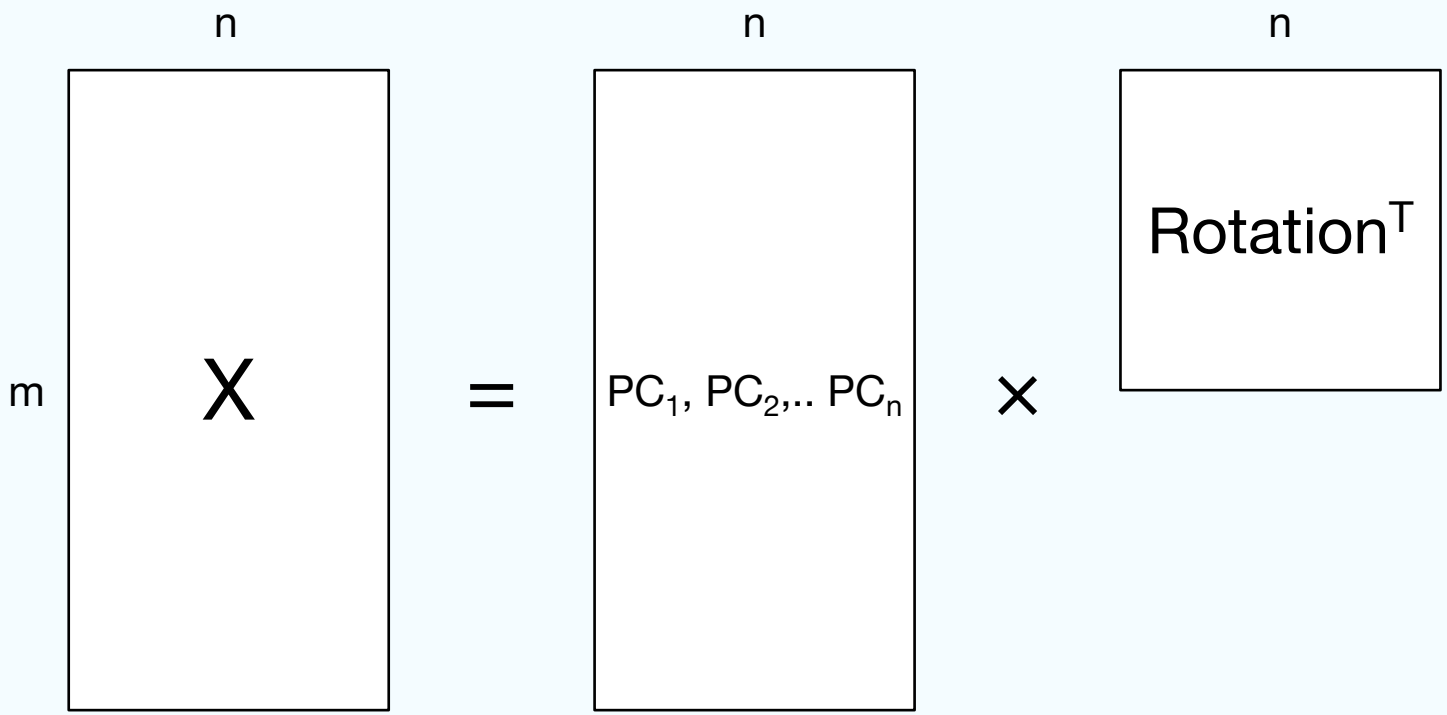
$$X = U\Sigma V^T$$

- The diagonal elements of Σ (i.e., λ_i) are **the square root of the eigenvalues** of $X^T X$, and columns of V are its **eigenvectors**.

- **PCA**
  - **The PCA score of X is $U\Sigma$, the rotation is V.** Contributions of each PC are equal to the relative proportion of λ_i.

PCA

- **PCA**
  - **The PCA score of X is $U\Sigma$, the rotation is V.**



PCA

- **Dimension reduction**

$$X = U\Sigma V^T$$

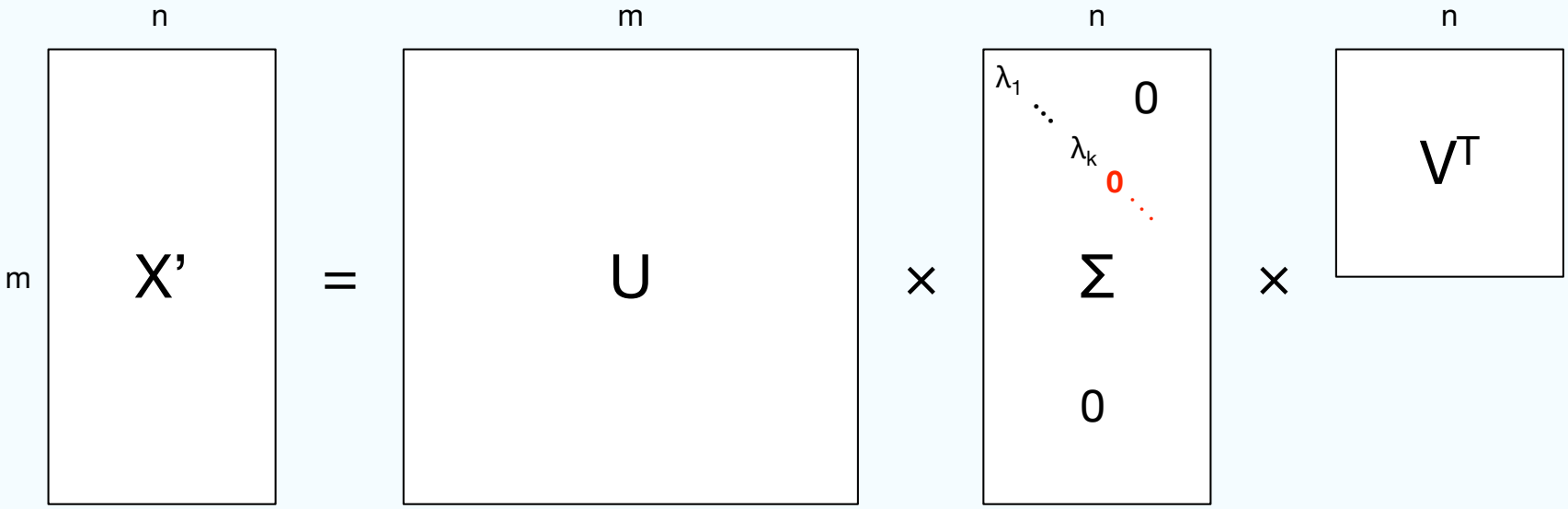
  - The diagonal elements of Σ is given by λ_i. and assume that they are in decreasing order.
  - Consider to approximate X by a lower dimension $k < n$, the approximation X' can be given by

$$X' = U\Sigma' V^T$$

    where Σ' is the same as Σ except $\sigma_{ii} = 0$ if $i > k$.

PCA

- **Dimension reduction**
  - By definition, all $\lambda_i > 0$. Let λ_i be in decreasing order.
  - Ignoring smaller λ_i $(i > k)$, X' will be an approximation of X.



Sequential Data Analysis

（系列データ解析）

SDA

- **Modeling time evolution**
  - Filters
  - Fourier Transform, Wavelet
  - Gaussian Process
  - Markov Chain
  - Ordinal differential equations, Stochastic differential equations
  - Data assimilation etc…

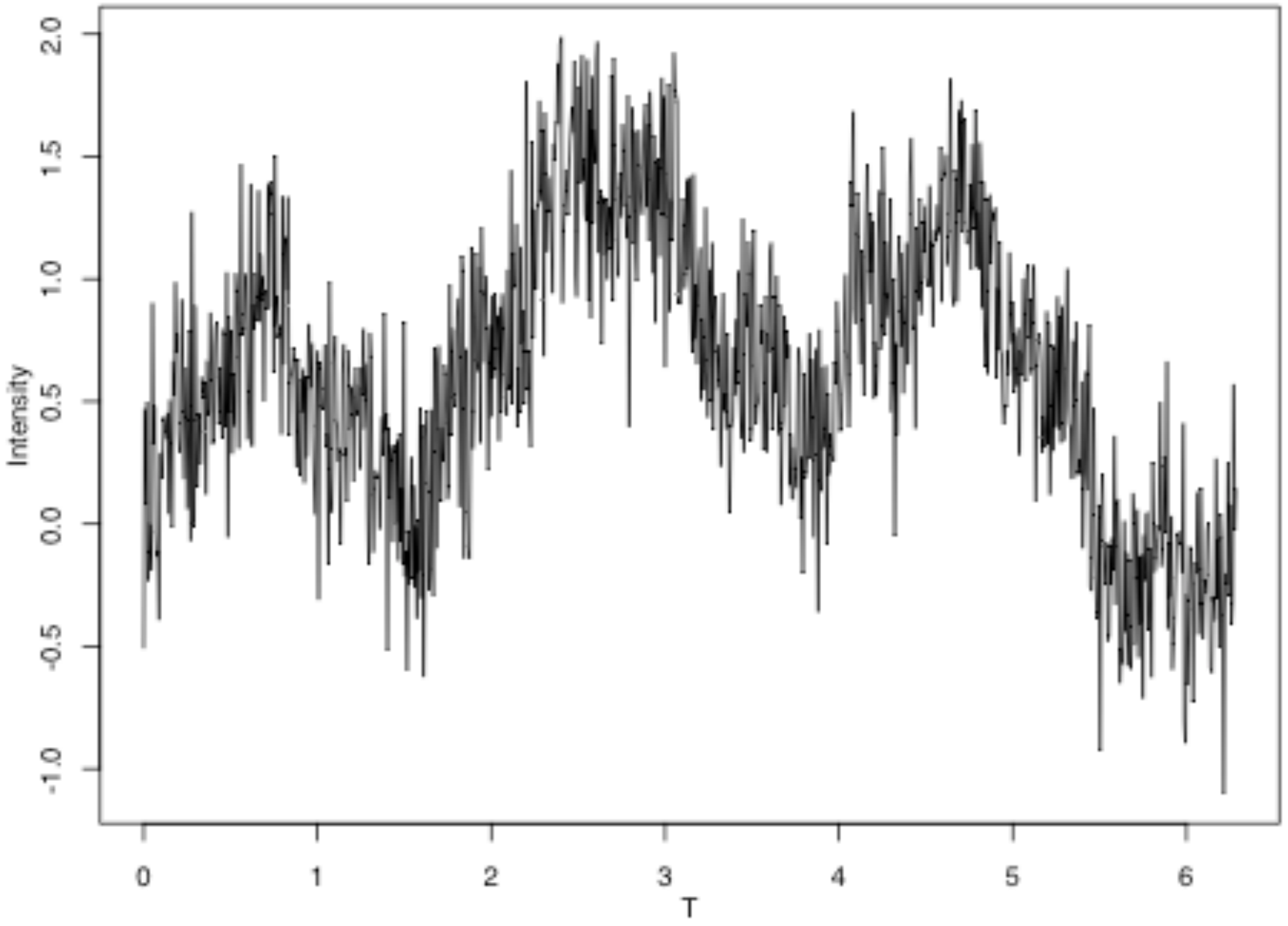
SDA

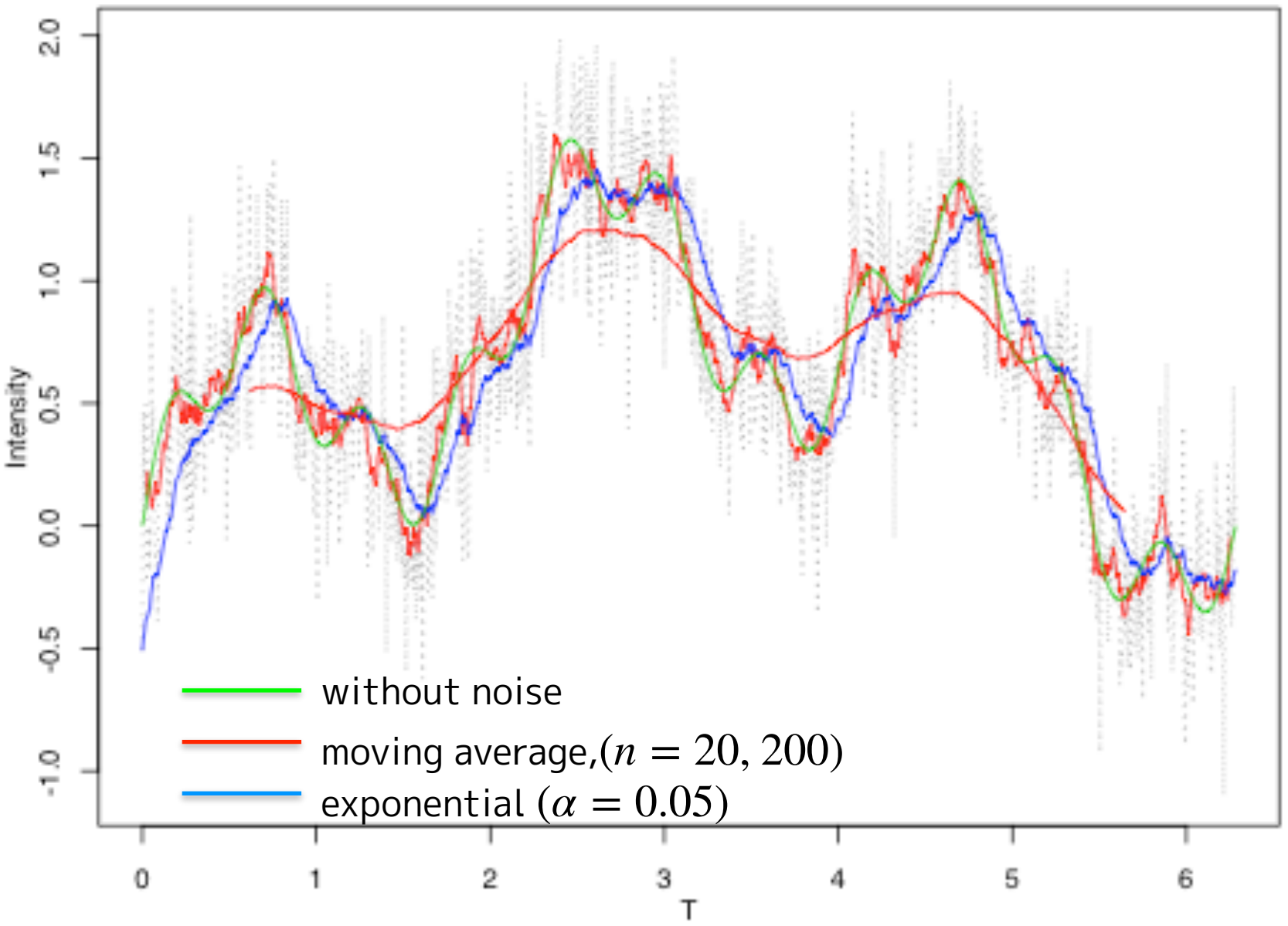
- **Moving Average Filter**
  - When the time series is noisy, moving average would reduce the effect of random fluctuation.

$$x_{MA}(t) = \frac{1}{n}\sum_{\tau=0}^{n-1} x(t-\tau)$$

- **Exponential Average Filter**

$$x_{EA}(t) = \lambda x(t) + (1-\lambda)x_{EA}(t-1)$$


Intensity
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
0
1
2
3
4
5
6
T

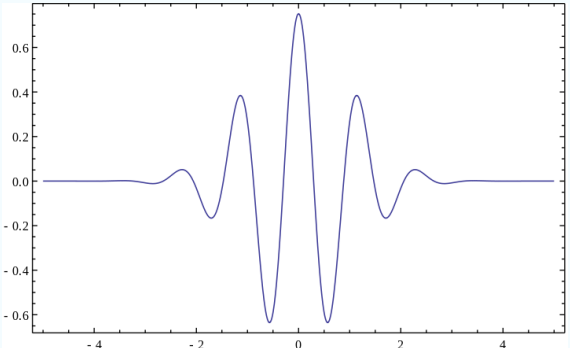

Intensity
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
0
1
2
3
4
5
6
T
without noise
moving average,($n = 20, 200$)
exponential ($\alpha = 0.05$)

SDA

- **Feature Analysis**
  - Fourier Transform

    Compute power dependance on wave length, i.e., to find **periodic patterns** by convolution with triangular functions.
  - Wavelet Transform

    Like FT, but consider dependance on both wave length and position using **wavelet mother functions.**

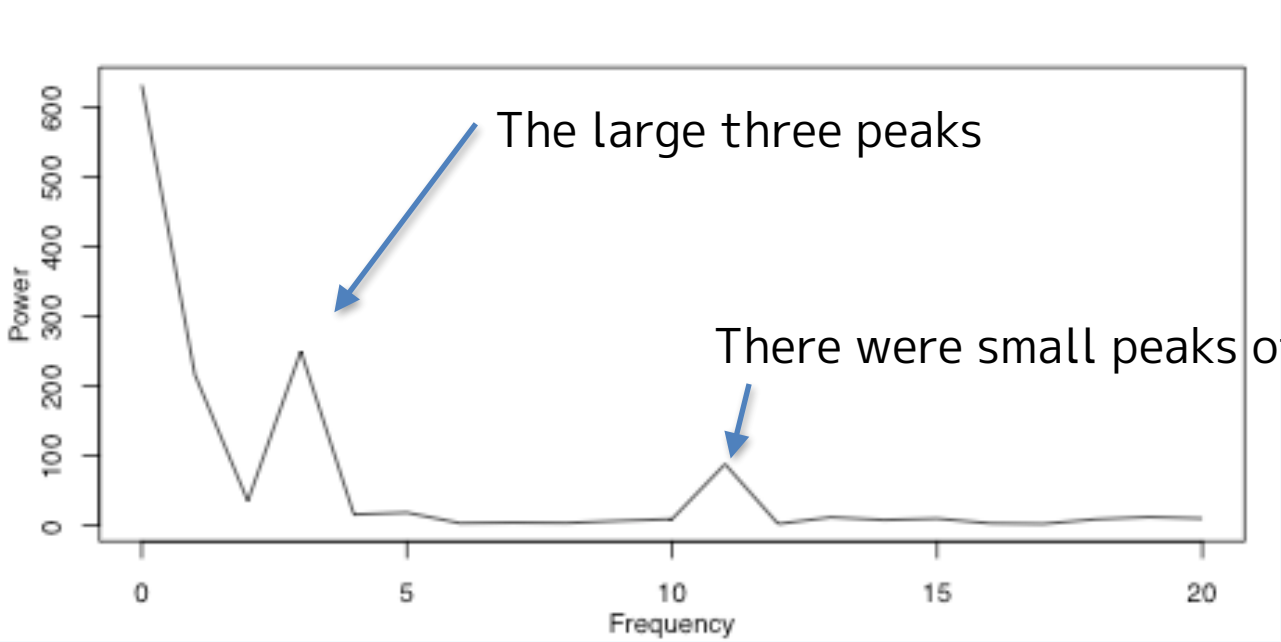


SDA

- **Fourier transform**

Continuous : $F(k) = \int f(x) e^{-2\pi i k x} dx$

Discrete : $F_k = \frac{1}{N} \sum f_j e^{-2\pi i j k / N}$

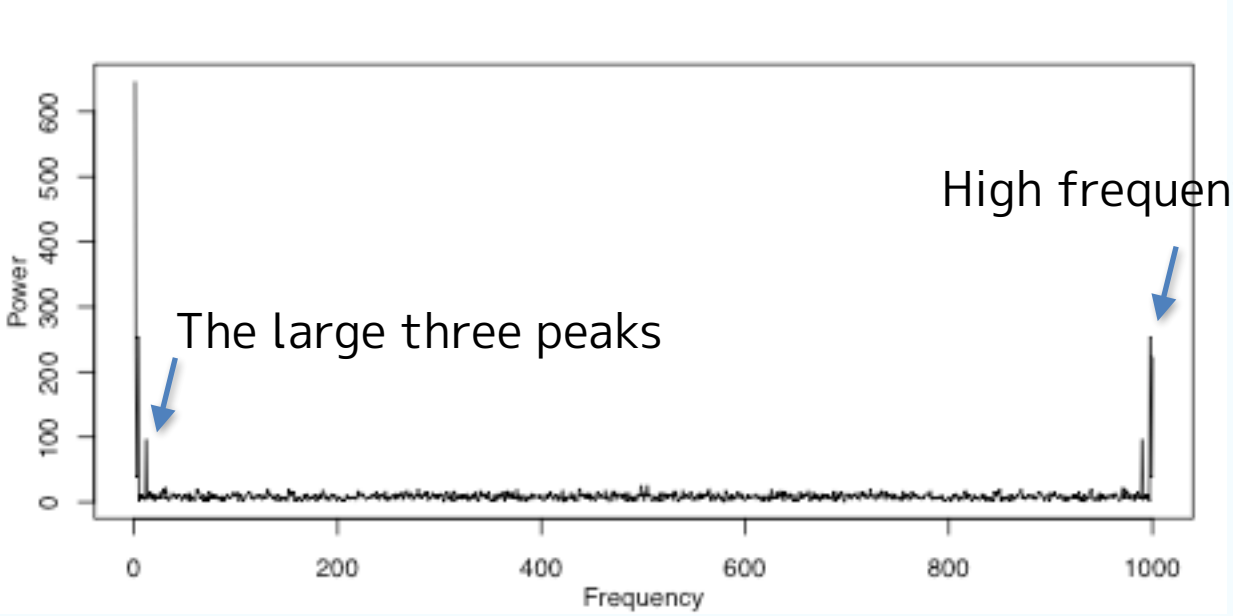


SDA

- **Fourier transform**

$$\text{Continuous} : F(k) = \int f(x) e^{-2\pi i k x} dx$$

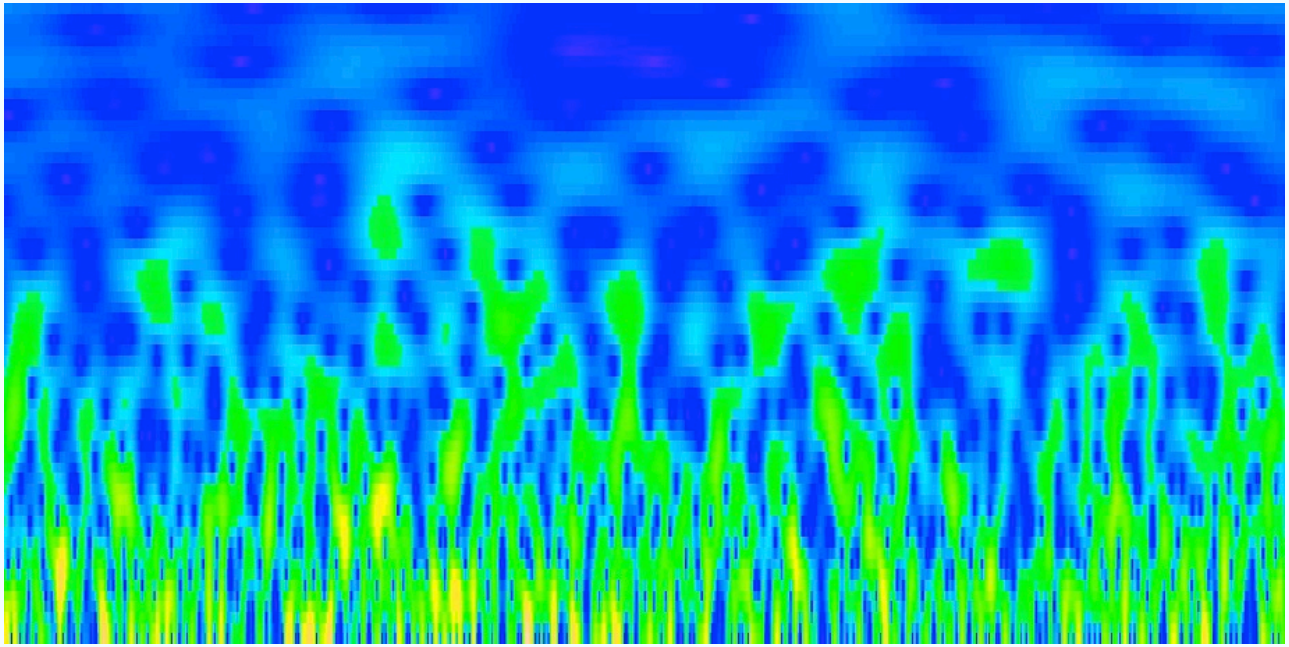
$$\text{Discrete} : F_k = \frac{1}{N} \sum f_j e^{-2\pi i j k / N}$$



SDA

- **Wavelet Transform**

$$\Phi(k, x') = \int \frac{1}{\sqrt{k}} f(x) \phi(\frac{x - x'}{k}) dx$$



The X and Y axis denote position of waves and wave length.
The hue from blue to white represents the power at (k, T)

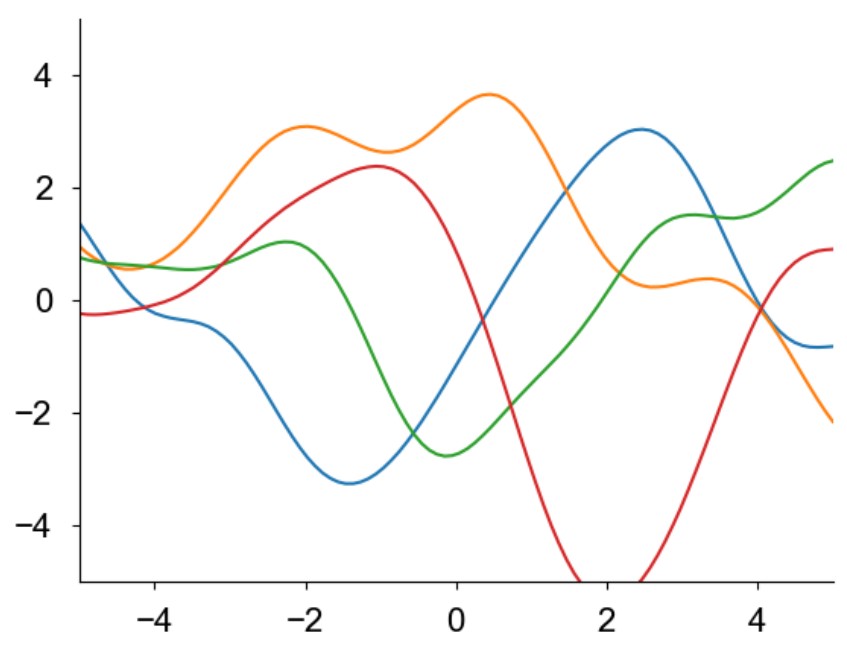
SDA

- **Gaussian Process (GP)**
  - Consider a generalized linear regression using Radial Basis Function (RBF), i.e., Gaussian.

$$f(x) = \int \phi(x') e^{-\frac{(x - x')^2}{\sigma^2}} dx'$$

GP is a probabilistic model of $f(x)$.

Assuming a prior distribution of $\phi(x)$, we can model a wide range of samples of $f(x)$ that belongs to the GP.



Samples from the GP. The smoothness of the curves depends on the σ.

SDA

- **Gaussian Process Regression**
  - Given a set of observation X, Y, we can evaluate posterior distribution of the GP using a kernel trick.
  - The posterior of y at a given x' is a Gaussian, as follows

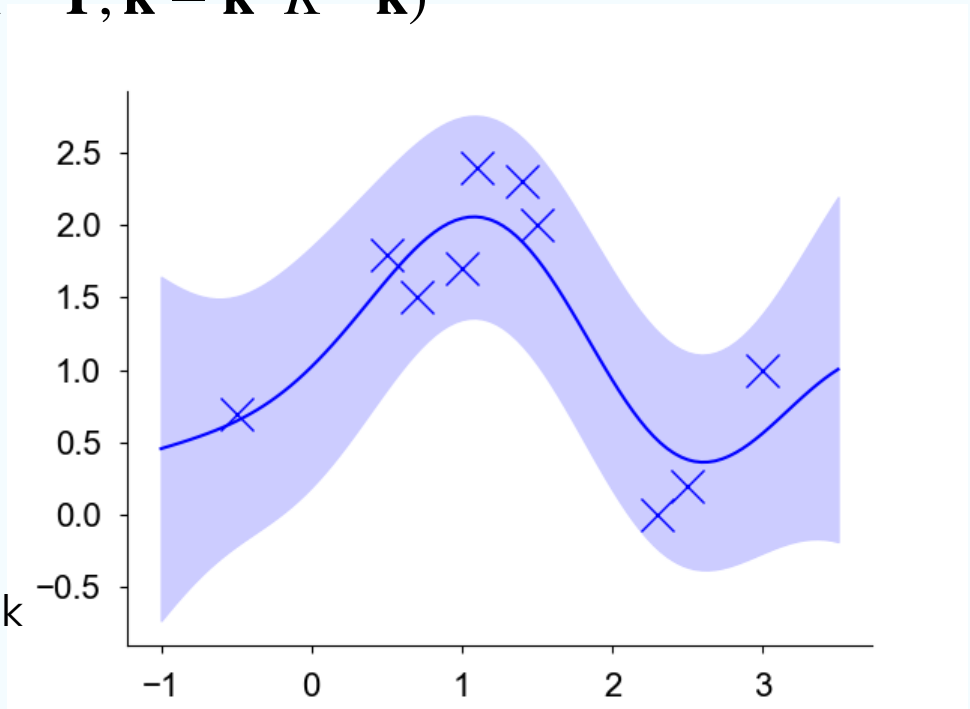
$$p(y(x \mid x') \mid \mathbf{X}, \mathbf{Y}, \theta) \sim N(\mathbf{k}^T K^{-1} \mathbf{Y}, \mathbf{k} - \mathbf{k}^T K^{-1} \mathbf{k})$$

where

$$k(x_1, x_2) = e^{-\frac{(x_1 - x_2)^2}{\theta^2}}$$

$$K = k(\mathbf{X}, \mathbf{X})$$

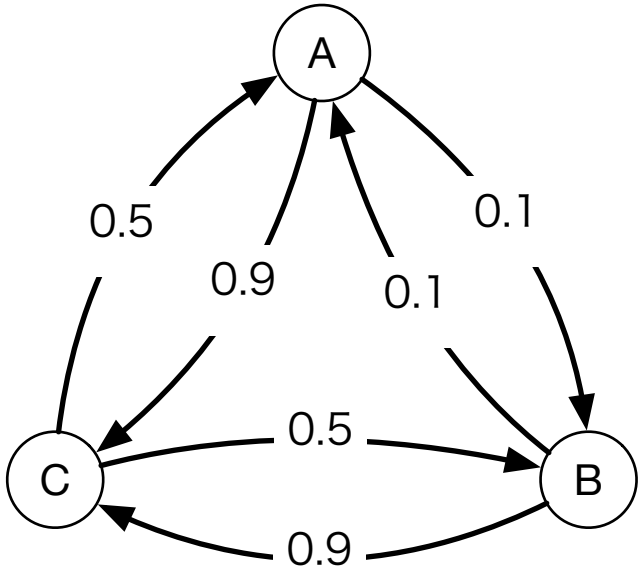
$$\mathbf{k} = k(x', \mathbf{X})$$



An example of GP regression. The blue line is the average and the dark region shows SD of the prediction

SDA

- **Markov Chain**
  - Memoryless discrete random process between finite states.
  - Defined by a transition probability matrix.



$$P = \begin{bmatrix} 0 & 0.1 & 0.9 \\ 0.1 & 0 & 0.9 \\ 0.5 & 0.5 & 0 \end{bmatrix}$$

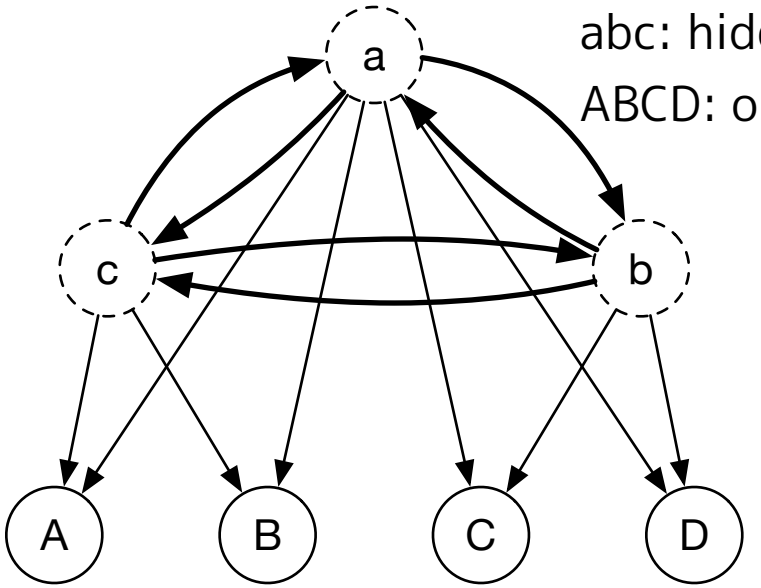
Sample State Sequence: A,C,A,B,C,B,C,B,C,B,...

SDA

- **Hidden Markov Model**
  - Markov models with unobservable ("hidden") states.
  - Observations Y depends on the hidden states X.

$$P(Y) = \sum_{X} p(Y|X)p(X)$$

Hidden states and their transition probability matrix can be estimated from the sequence of observations using Bayesian inference.



abc: hidden states

ABCD: observations

Deep Learning （深層学習）

Deep Learning

- DL is a one of the architectures of artificial neural networks.

- **Artificial Neural Networks**
  - Perceptron
  - Three Layer ANN
  - Deep Neural Networks
  - Convolutional Neural Networks
  - Recurrent Neural Networks

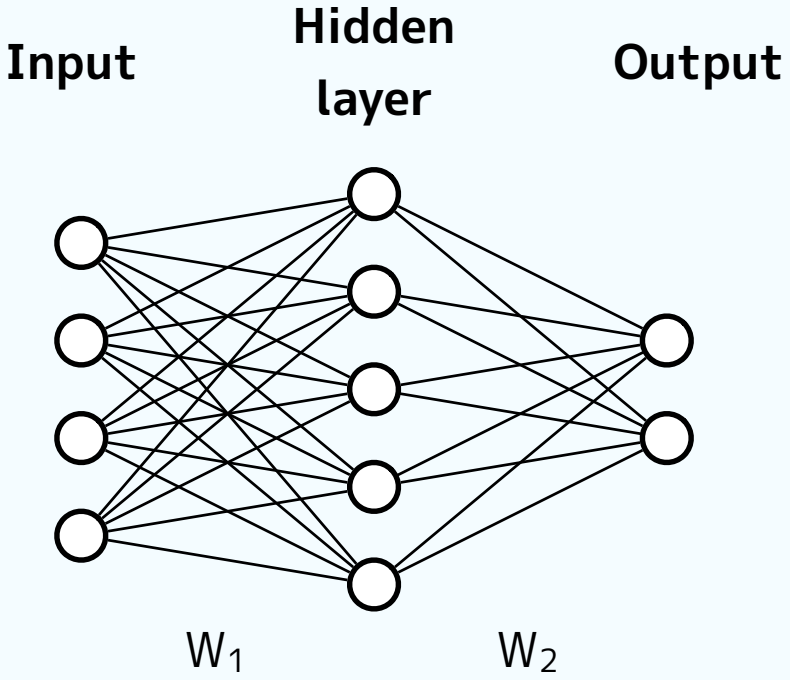
Deep Learning

- **Perceptron**
  - The output of a layer in perceptron is given as follows,
  - $\mathbf{x}_{l+1} = W_l \mathbf{x}_l + \mathbf{b}_l$

    $\mathbf{x}_l$ is the input, W_l is the weight matrix, and $\mathbf{b}_l$ is the bias.
- **Artificial Neural Networks**
  - $\mathbf{x}_{l+1} = f\left(W_l \mathbf{x}_l + b_l\right)$
  - Generally some non-linear activation function is applied to the output of ANN.

Deep Learning

- **Artificial Neural Networks**
  - A simplest architecture of an artificial neural network is three layer neural networks,



x_1: Input

$v_2 = W_1 x_1 + b_1$

$x_2 = f(v_2)$: Hidden

$v_3 = W_2 x_2 + b_2$

$x_3 = f(v_3)$: Output

Deep Learning

- **Training**
  - We need to optimize the weight parameters to obtain desirable models.
  - Minimize "loss" function, for example,

    Mean squared error: $L_2(\mathbf{y}, \mathbf{y}') = \frac{1}{N} |\mathbf{y}' - \mathbf{y}|^2$

    Cross entropy: $L_X(\mathbf{t}, \mathbf{p}) = -\sum t_i log(p_i)$
  - Gradient descent

    The most general stepwise optimization method.

    $W^{t+1} = W^t - \lambda \nabla L(\mathbf{X}; W^t)$

Deep Learning

- **Back propagation**
  - To optimize all W_l, we can compute their derivative using the **chain rule**, though it looks complicated …

$$\frac{\partial L}{\partial W_n} = \frac{\partial L}{\partial \mathbf{y}_n}\frac{\partial \mathbf{y}_n}{\partial W_n} = \frac{\partial L}{\partial \mathbf{y}_n}\frac{\partial \mathbf{y}_n}{\partial \mathbf{x}_n}\frac{\partial \mathbf{x}_n}{\partial W_n} = L'(y_n)f'(x_n)W_n(\mathbf{x}_{n-1})$$

$$\frac{\partial L}{\partial W_{n-1}} = \frac{\partial L}{\partial \mathbf{y}_n}\frac{\partial \mathbf{y}_n}{\partial \mathbf{x}_n}\frac{\partial \mathbf{x}_n}{\partial \mathbf{y}_{n-1}}\frac{\partial \mathbf{y}_{n-1}}{\partial \mathbf{x}_{n-1}}\frac{\partial \mathbf{x}_{n-1}}{\partial W_{n-1}} = \sum_i L'(y_n)f'(x_n)W_n x_{n-1,i} f'(x_{n-1})W_{n-1}(x_{n-2})$$

$$\vdots$$

Deep Learning

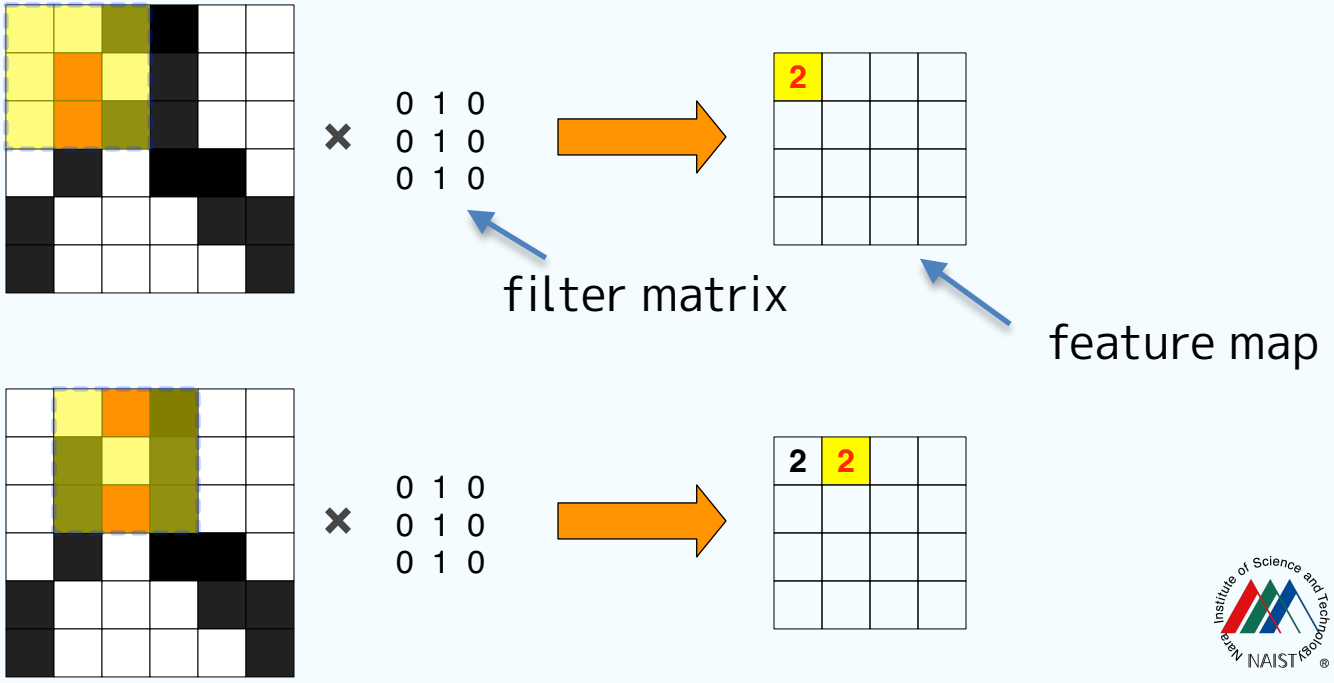
- **Three layers architecture of ANN**
  - Many layers ANN implies smaller gradients.

    > optimization will become difficult and slower.
  - Theoretically, three-layers ANN can compute arbitrary boundaries. (if the number of nodes are large enough)

    > Deeper ANN had not been studied so much.
- **Deep Learning**
  - Recently, "Big Data" and higher computational power allow us to train more complex ANNs.

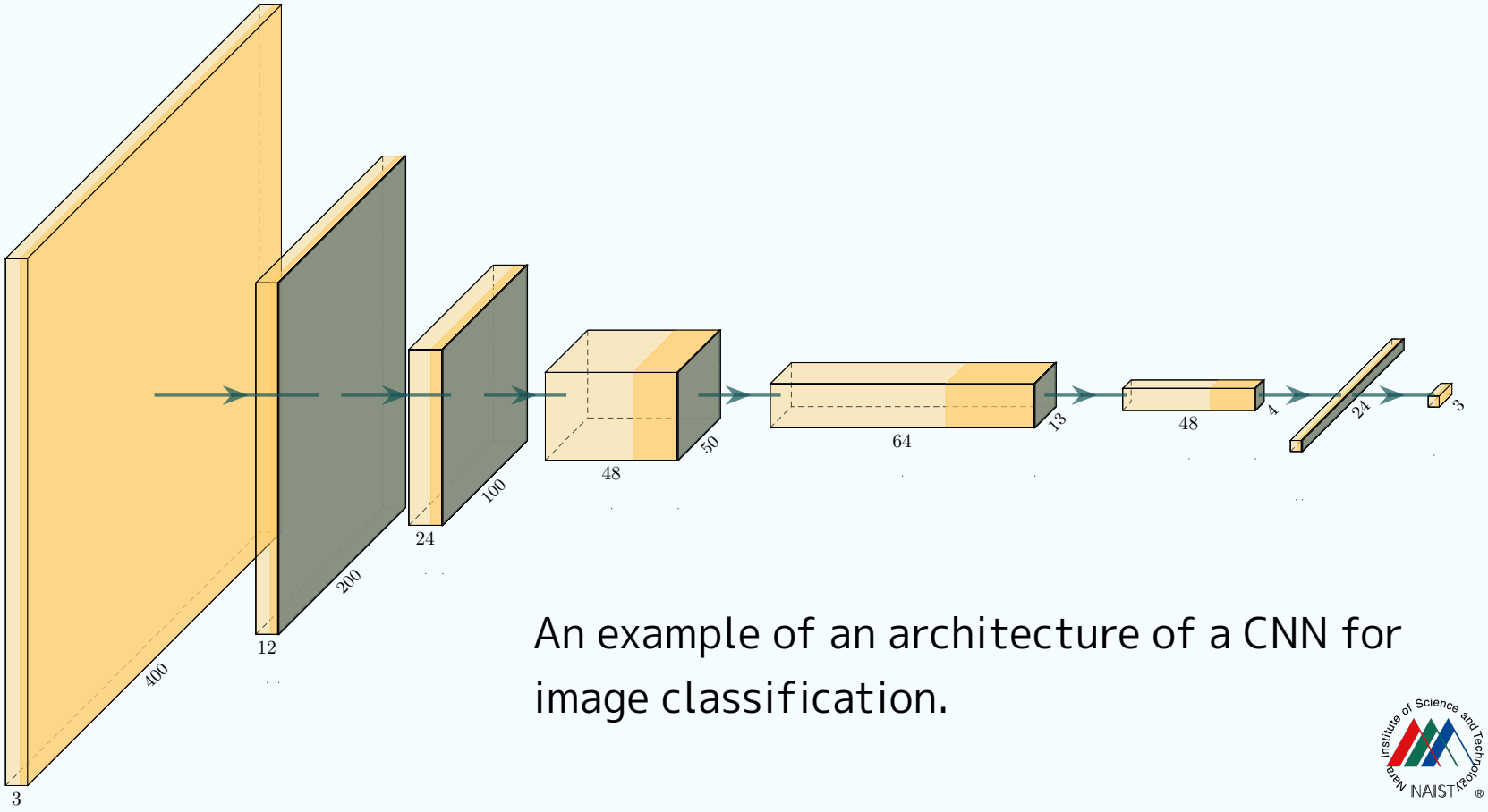
Deep Learning

- **Convolutional Neural Networks**
  - Like as wavelet, convolution using weighted "filter" extracts local feature from given images.
  - Optimizing recursive filters allows us to obtain more complex features.



CNN

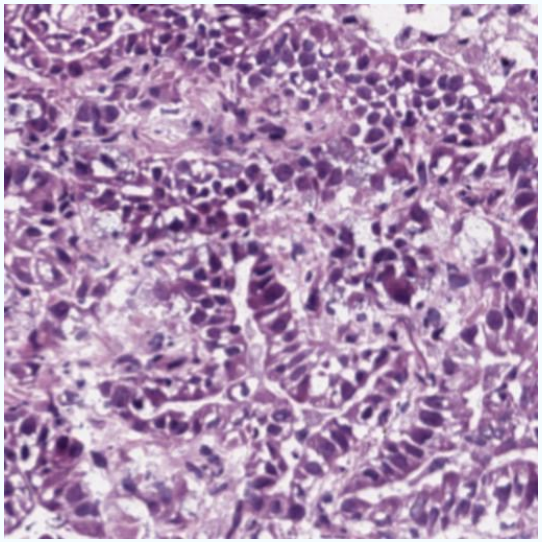
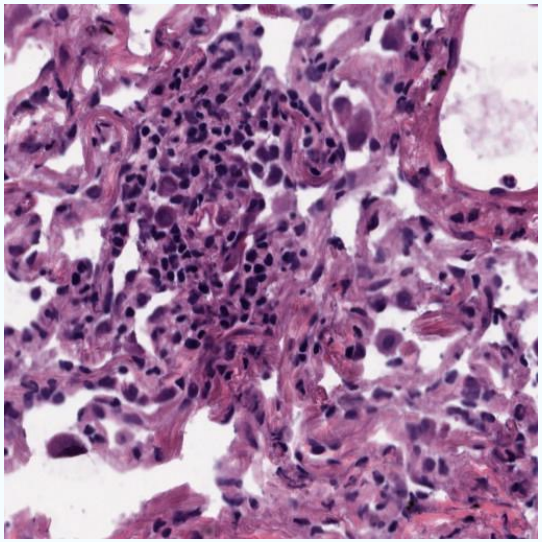
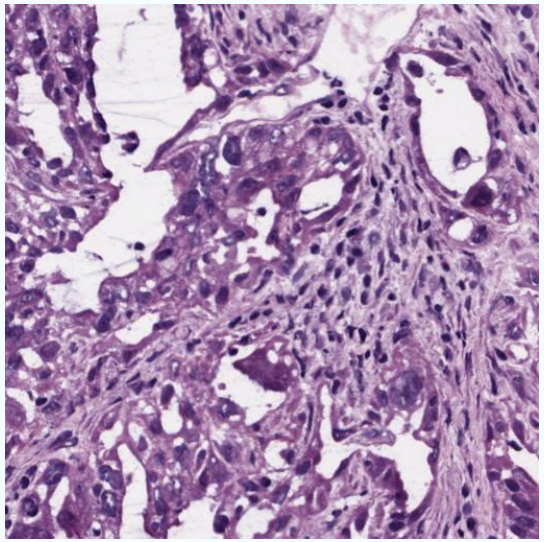
- **Image classification using CNN**
  - Extracting features from pixel matrix using layers of convolution and converged to the output nodes.



An example of an architecture of a CNN for image classification.

CNN

- **Image classification using CNN**
  - CNN can distinguish three sub-types of lung cancer from pathological images with 98.9% accuracy.

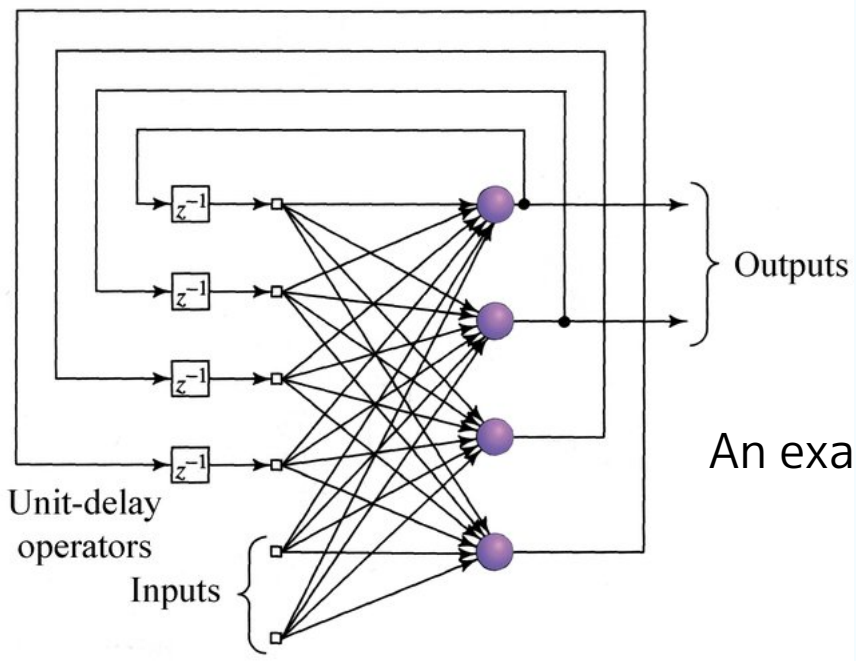




Sections of pathological images of thee subtypes of lung cancer.

[Antonio et al. IJCARS 2018]

Deep Learning

- **Recurrent Neural Networks**
  - Concatenating some output with the next input, an ANN can memorize its inner states.
    > Useful to extract features from sequential data.



An example of an architecture of an RNN

Deep Learning

- **Application of Deep Neural Networks**
  - Classifier

    Train to output discrete target variables.
  - Regressor

    Train to output continuous target variables.
  - AutoEncoder

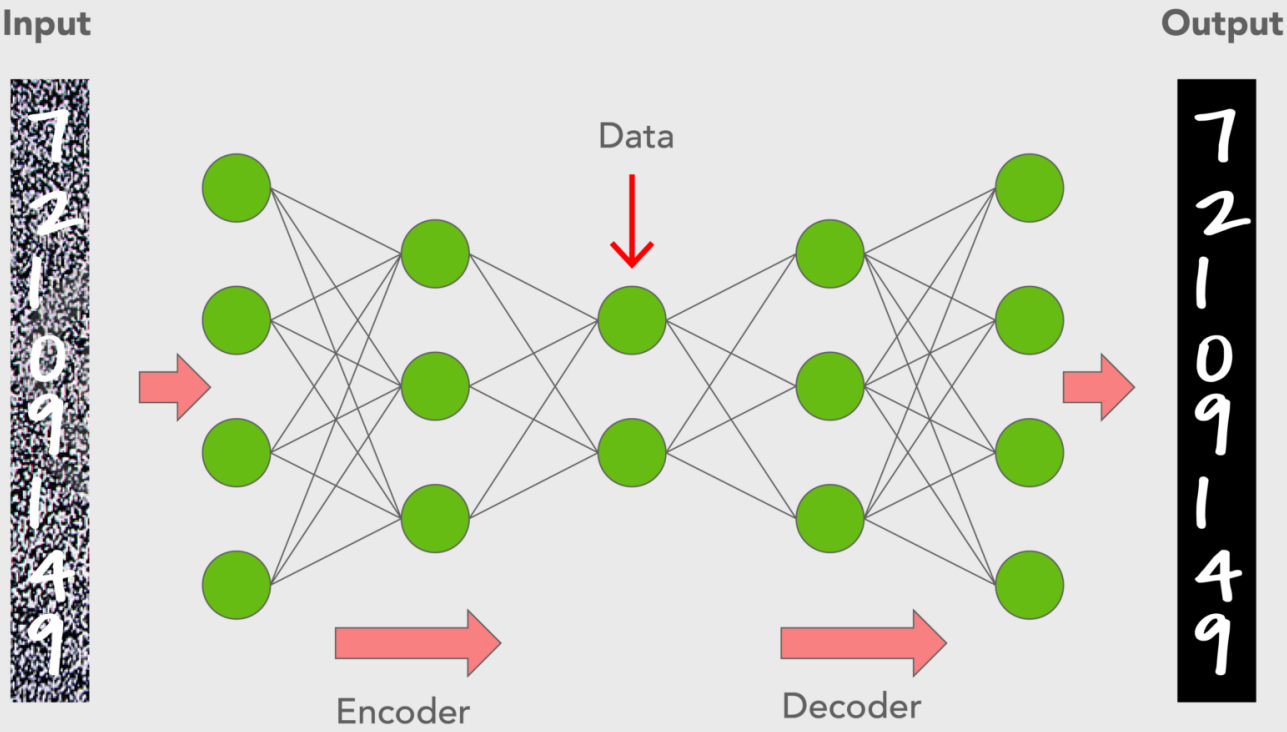
    Train to reconstruct the input using smaller features.
  - Converter

    Train to generate output from extracted features.
  - Generator

    Train to generate from some small parameters.

Deep Learning

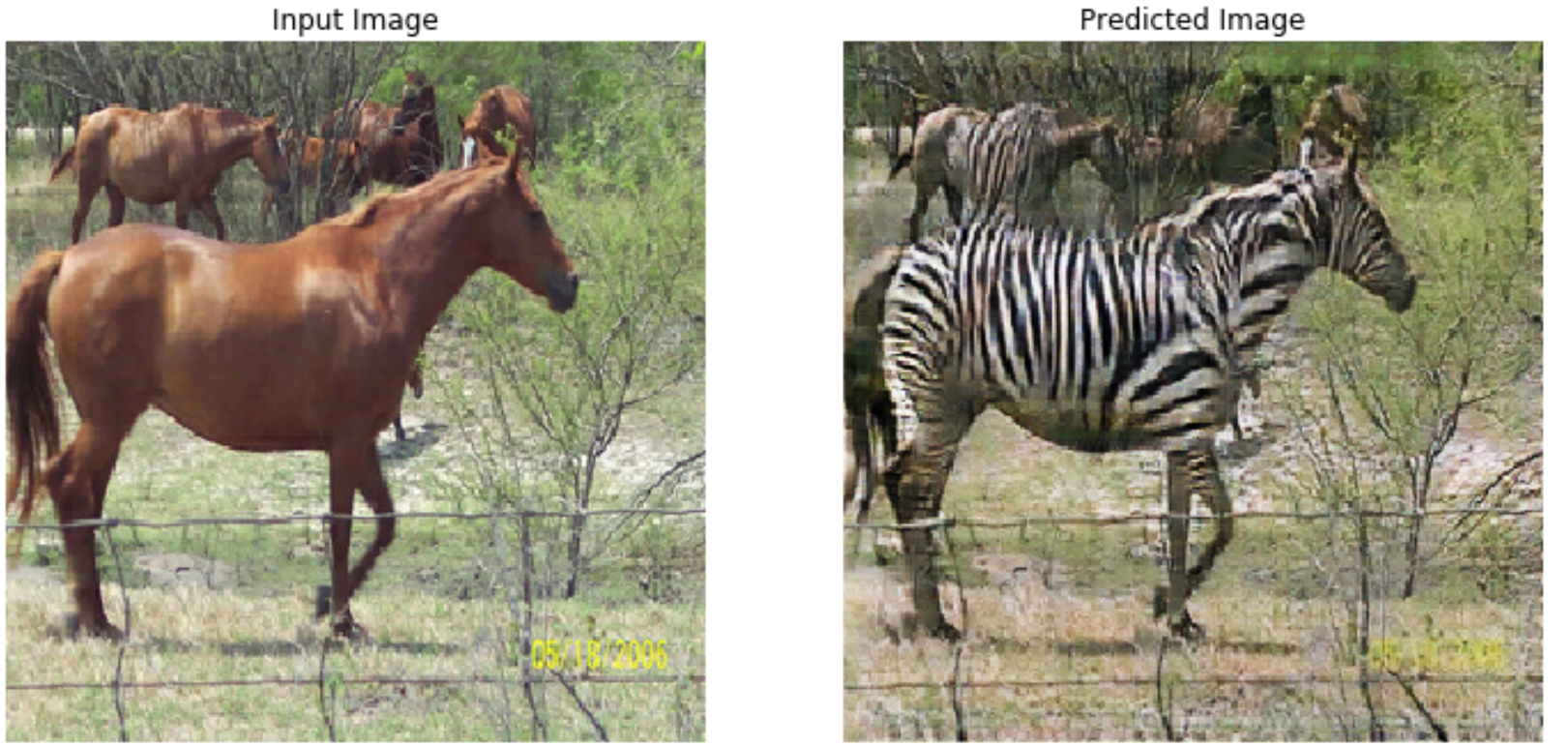
- **Autoencoder**
  - Train both encoder and decoder to reconstruct inputs.



A schematic illustration of an architecture of a Denoising autoencoder.
By training to extract feature of digits, it can reduce unrelated noises.

Deep Learning

- **Converter**
  - Train encoder and decoder to construct new images.



An example of image translation using CycleGAN.

[https://arxiv.org/abs/1703.10593]

Deep Learning

- **Generator**
  - Construct a decoder from latent space.

Generated images using StyleGAN

[NVIDIA research paper at ICLR 2018]

Model Selection

Model Selection

- **Measure of distribution**
  - Evaluate distance between true sample distribution ($p(x)$) and predicted probability distribution ($q(x)$).
  - Distance (L2):

$$D(p,q) = \int |p(x) - q(x)|^2 dx$$

  - Kullback–Leibler divergence:

$$KL(p||q) = \int p(x) \log \frac{p(x)}{q(x)} dx$$

both D and KL become minimum and equal to 0 iff $p(x) \equiv q(x)$

Model Selection

- **Kullback–Leibler divergence:**

$$KL(p||q) = \int p(x)\log\frac{p(x)}{q(x)}dx$$

$$= \int p(x)\log p(x)dx - \int p(x)\log q(x)dx$$

(negative) Entropy of $p(x)$ Mean log likelihood

When $p(x)$ is the distribution of sample X,

$$= -S(X) - E_X[L(q)] \qquad x \in X$$

where $S(X)$ is the entropy, $L(q)$ denote log likelihood,

$E_X[]$ is the expected value sampled from X.

Model Selection

- **Mean Log Likelihood**
  - Consider a model with parameters $q(x;\alpha)$

    When the model is the best, $KL(p||q(\alpha))$ is minimum.

    Though generally, we don't know $p(x)$ to estimate KL.

$$KL(p||q(\alpha)) = -S(X) - E_X[L(q(\alpha))]$$

S does not depend on α

Maximize MLL

And according to the "law of large numbers",

$$E_X[L(q(\alpha))] = \lim_{N\to\infty} \frac{1}{N} \sum_i \log q(x_i;\alpha)$$

We no longer need to know $p(x)$, if the sample size is large enough.

Model Selection

- **Information Criteria**
  - We can approximately evaluate MLL and find the parameter that maximize it.

    Note: When we estimate α from the observed samples, there remains a **bias** that reduce L compared to the true distribution.
  - Akaike Information Criteria

$$AIC = -2\log(\hat{L}) + 2k \sim -2MLL$$

  - Bayesian Information Criteria

$$BIC = -2\log(\hat{L}) + k\log n \sim -2MLL$$

The constant "-2" derived from a historical background.

Model Selection

- **Leave One Out Cross Validation**
  - LOOCV can be regarded as an approximation of MLL.
    > Smaller LOOCV is equivalent to smaller MLL.
- **Model comparison**
  - Though we do not know $S(X)$, it is constant. We can compare relative difference of MLL, i.e., log likelihood ratio (LLR) **to select better model**.
  - Most of **statistical tests** can be regarded as comparison of LLR to that of "null model".

-log(p-value) generally correlates with LLR in statistical tests.

Afterwords

- **Modeling and Learning**
  - Why we need models?

    To predict future observation from past observed sample data.
  - What is "learning" in data science?

    Construct a model with adjustable parameters, then find their optimum to improve prediction accuracy.
  - How can we know which modeling is better?

    By measuring difference between predicted and observed probability distribution.

Report

Report

- **Task**
  - You have thousands samples of multivariate (less than 100 dimensions) observations. Discuss about a method how to separate 'noise' component from the data and how to evaluate appropriateness of the method.

    Hint: Propose arbitrary models (either linear or non-linear).
  - **Words:** less than 500 words (about A4 1page)
  - **Language:** English or Japanese (日本語でも可)

    Note: You may refer textbooks and web pages, and must cite all references properly.

The word count does not include the references.

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- **課題**
  - 数千件、数十次元の多次元のサンプルデータの配列があるものとする。このデータから「ノイズ成分」を分離する方法について、またその方法を評価する手法について議論せよ。

    ヒント: なんらかの具体的なモデルを（線形でも非線形でも）提案し、そのモデルに基づいて考察すること。
  - **分量:** 1500 字 (A4 1ページ) 以下
  - **言語:** 日本語でも可

    注: 教科書やwebサイトを参考にしても構わないが、参照した文献をすべて適切に引用すること。

    （引用及び図表は分量に含まない）

Report

- **Submission**
  - Open the NAIST online syllabus.

    https://syllabus.naist.jp/subjects/preview_detail/621
  - Find the link to the DropBox and open it.

    Password: naist2020ds
  - Drop you file via your web browser.
  - **Name your report file as follows,**

    3_{StudentID}_{LastName}_{FirstName}.pdf

    (example: 3_0105072_Ono_Naoaki.pdf)
  - **Keep the deadline.**

    2020/6/26, 23:59