Konstruksjon av høydimensjonale nevralt nettverk-potensialer for molekylærdynamikk

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Hva er molekylærdynamikk?

- Numerisk metode for å simulere atomers og molekylers bevegelser i gasser, væsker og faste stoffer.
- Virtuelt eksperiment.

Dynamikk

- Partiklenes interaksjoner styrer dynamikken.
- Interaksjonene bestemmes av et kraftfelt **F**:

$$\mathbf{F} = -\nabla V(\mathbf{r})$$

- Potensiell energiflate / potensial):

$$V(\mathbf{r}), \quad \mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$$

- $V(\mathbf{r})$ inneholder all fysikken.

Ab inito molekylærdynamikk

Løse Schrödinger-likningen ved hvert tidssteg.

Klassisk molekylærdynamikk

Bruke en predefinert analytisk funksjon.

Klassisk potensial

$$V(\mathbf{r}) \approx \sum_{i}^{N} V_1(\mathbf{r}_i) + \sum_{i,j}^{N} V_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i,j,k}^{N} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$

Hvordan bør leddene se ut?

Eksperiementer / kvantemekanikk

"Fysisk" strategi:

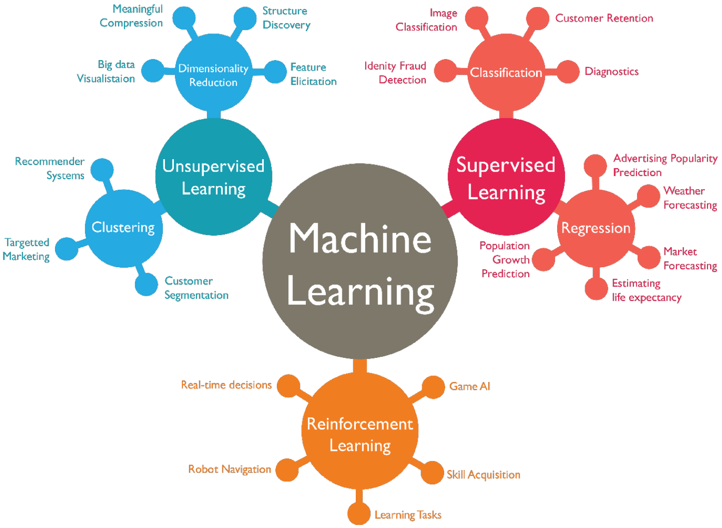
1. Starte med en funksjonsform med noen parametre.
2. Bestemme parametre fra eksperimentelle data.

"Matematisk" strategi:

1. Produsere kvantemekaniske data.
2. Tilpasse en generell funksjonsform til dataene.

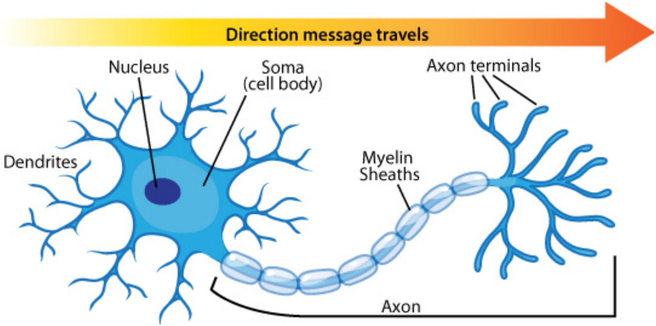
Interpolere datasett

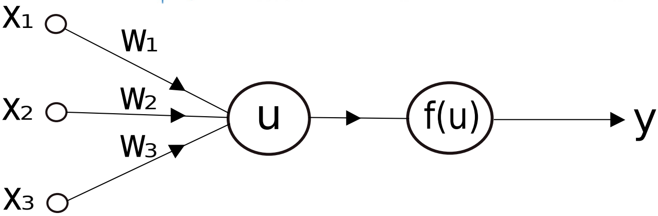
- Spliner
- Minste kvadraters metode
- Maskinlæring

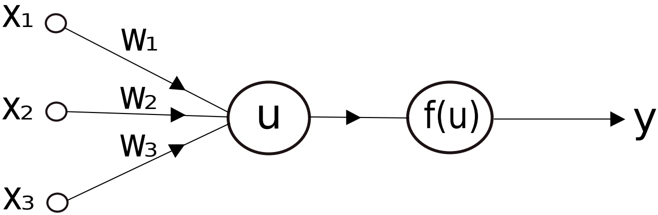

Machine Learning
Unsupervised Learning
Dimensionality Reduction
Meaningful Compression
Structure Discovery
Big data Visualistaion
Feature Elicitation
Clustering
Recommender Systems
Targetted Marketing
Customer Segmentation
Supervised Learning
Classification
Image Classification
Customer Retention
Idenity Fraud Detection
Diagnostics
Regression
Advertising Popularity Prediction
Weather Forecasting
Population Growth Prediction
Market Forecasting
Estimating life expectancy
Reinforcement Learning
Real-time decisions
Game AI
Robot Navigation
Skill Acquisition
Learning Tasks

Kunstige nevrale nettverk

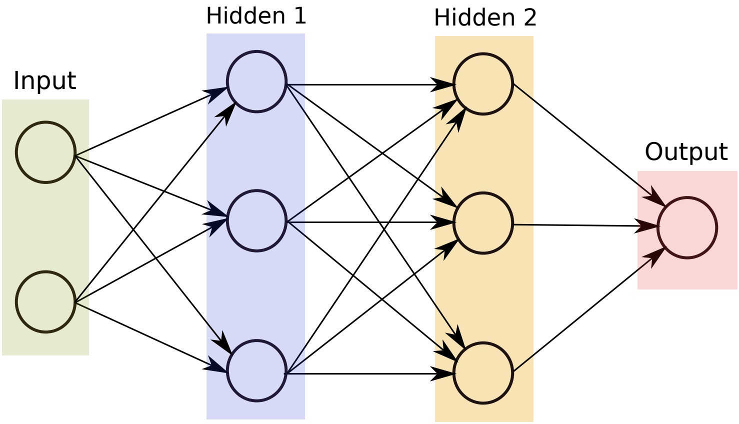
- Etterlikne en biologisk hjerne
- Nettverk av matematiske nevroner


Direction message travels
Nucleus
Soma
(cell body)
Axon terminals
Dendrites
Myelin
Sheaths
Axon

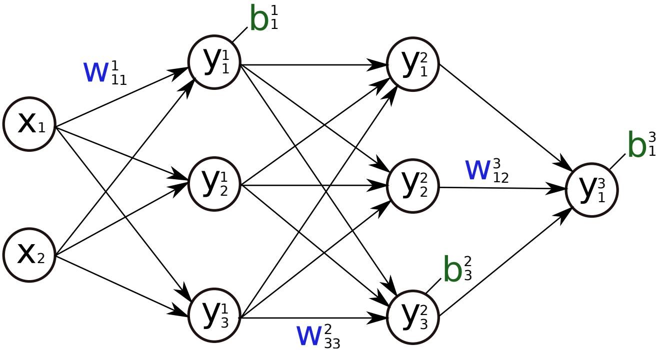

x1
w1
x2
w2
w3
x3
u
f(u)
y



$$y = f\left(\sum_{i=1}^{n} w_i x_i + b_i\right) = f(u)$$



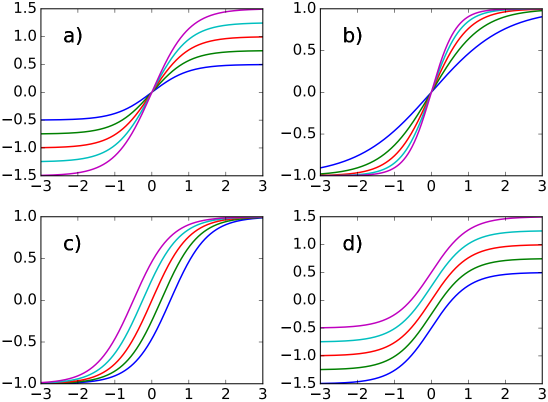
Input
Hidden 1
Hidden 2
Output



$$y_i^1 = f_1(u_i^1) = f_1\left(\sum_{j=1}^{2} w_{ij}^1 x_j + b_i^1\right)$$

$$y_1^3 = f_3\left[\sum_{j=1}^{3} w_{1j}^3 f_2\left(\sum_{k=1}^{3} w_{jk}^2 f_1\left(\sum_{m=1}^{2} w_{km}^1 x_m + b_k^1\right) + b_j^2\right) + b_1^3\right]$$

$$h(x) = c_1 f(c_2 x + c_3) + c_4$$



Matrix notation

$$y_i^2 = f_2\left(\sum_{j=1}^{3} w_{ij}^2 y_j^1 + b_i^2\right)$$

$$\vec{y}_2 = f_2(\mathrm{W}_2\vec{y}_1+\vec{b}_2) = f_2\left(\begin{bmatrix} w_{11}^2 & w_{12}^2 & w_{13}^2 \\ w_{21}^2 & w_{22}^2 & w_{23}^2 \\ w_{31}^2 & w_{32}^2 & w_{33}^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^1 \\ y_2^1 \\ y_3^1 \end{bmatrix} + \begin{bmatrix} b_1^2 \\ b_2^2 \\ b_3^2 \end{bmatrix}\right)$$

Activation functions

The sigmoid

$$f(x) = \frac{1}{1 + e^{-x}}$$

and the hyperbolic tangent

$$f(x) = \tanh(x)$$