Do androids dream of solving the sign problem ?

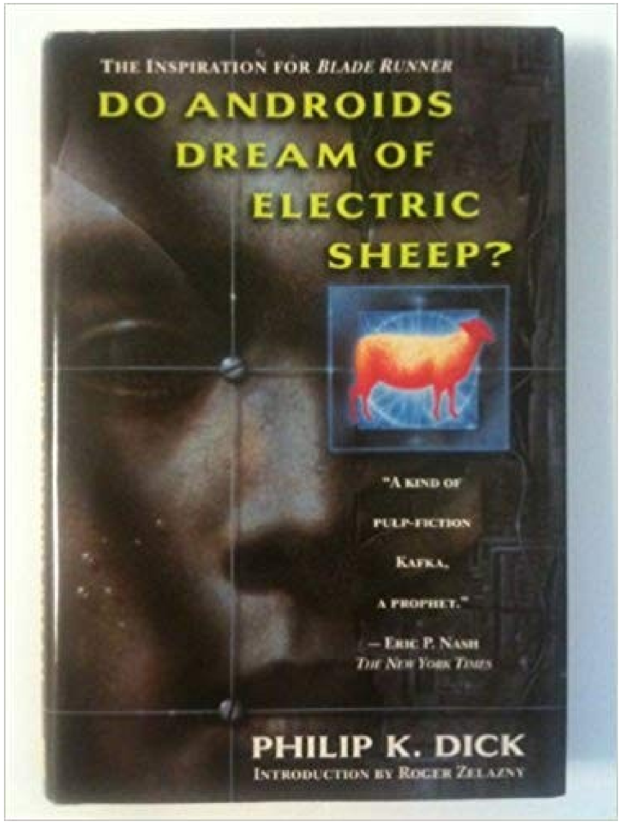
Akira Ohnishi (Nuclear theory group)

YITP Lunch Seminar, July 10, 2019

- **Outline**
  - **Androids and Neural Network**
  - **Sign Problem (Lefschetz thimble, Path Optimization)**
  - **Do neural network help us to search for the path ?**
  - **Summary**

Do androids dream of electric sheep ?

- **A novel by Philip K. Dick (1968), and the original of (inspiration for) the film, "Blade runner" (1982).**
- **Can androids (replicants) have emotion (humanity) ?**



P. K. Dick (1968)
(pic. from amazon)

Ridley Scott / Warner Bros
(pict. from amazon)

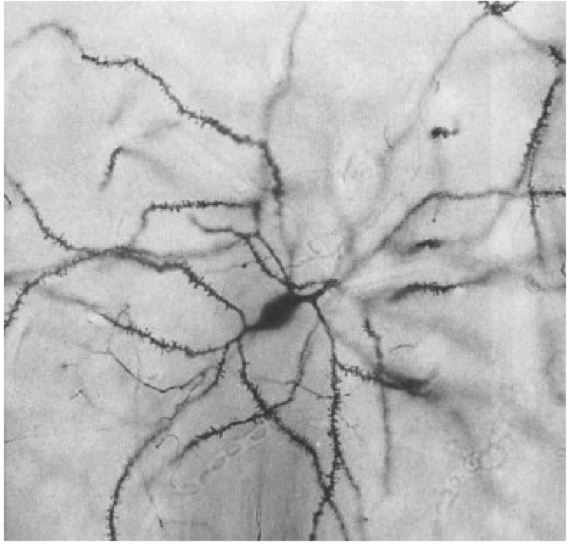
Neural Network

- **A mathematical model of brain, and the engine of androids (AI) and machine learning.**
- **Combination of linear and non-linear transf.**

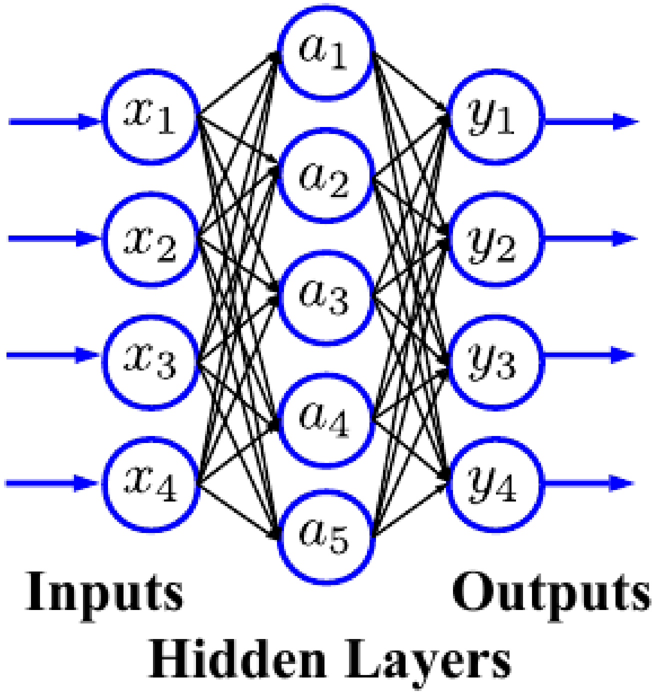
$$
\begin{aligned}
a_i &= g(\underline{W_{ij}^{(1)}} x_j + \underline{b_i^{(1)}}) \\
f_i &= g(\underline{W_{ij}^{(2)}} a_j + \underline{b_i^{(2)}}) \\
y_i &= \underline{\alpha_i} f_i + \underline{\beta_i} \\
g(x) &= \tanh x \ \text{(activation fn.)}
\end{aligned}
$$

variational parameters

- **Network parameters are optimized by using teacher data (pattern recog.), by try and error (board games), or to minimize the cost function.**



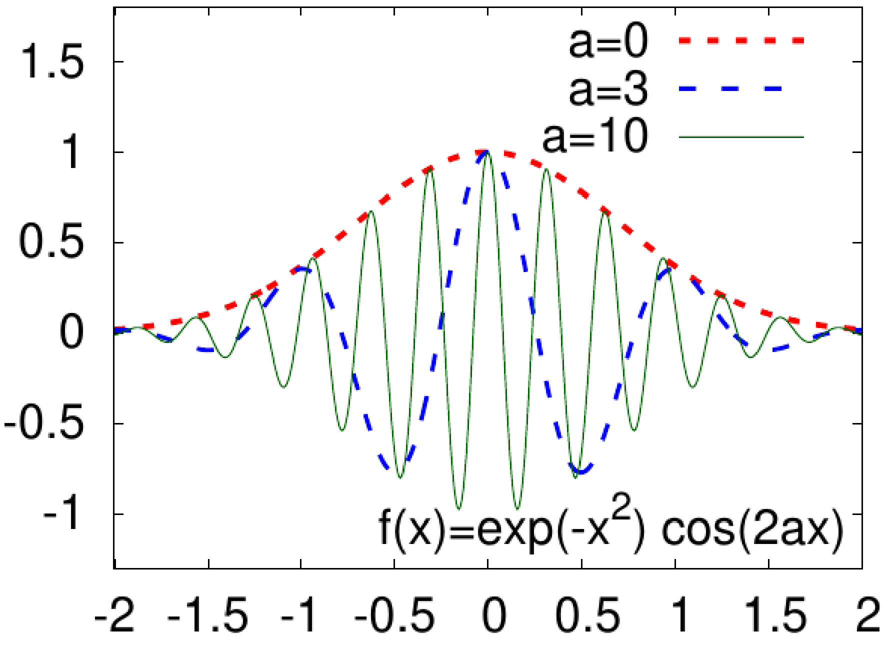
A. David Smith, J. P. Bolam, Trends in Neurosci. 13 ('90), 259

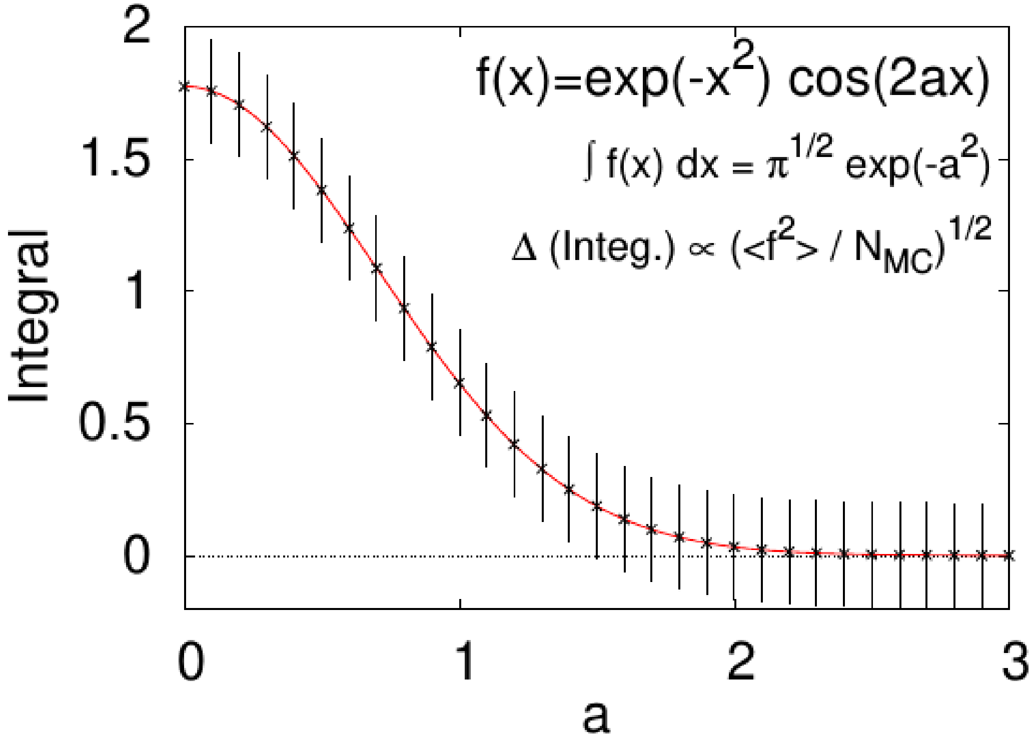


Sign problem

- **Numerical integration of oscillating function is difficult.**

$$\int dx\, \exp(-x^2)\cos(2ax) = \sqrt{\pi}\exp(-a^2)$$





We need Monte-Carlo samples $\propto$ exp(a^2)

Sign problem

- **Path integral with Complex Action S**

$$\langle\mathcal{O}\rangle=\frac{\int dx\ \mathcal{O}(x)e^{-S(x)}}{\int dx\ e^{-S(x)}}=\frac{\int dx\ \mathcal{O}(x)e^{i\theta}|e^{-S(x)}|}{\int dx\ \underline{e^{i\theta}}|e^{-S(x)}|}=\frac{\langle\mathcal{O}e^{i\theta}\rangle_{\mathrm{pq}}}{\underline{\langle e^{i\theta}\rangle_{\mathrm{pq}}}}$$

oscillation

$\propto \exp(-\#V)$

$$\langle\mathcal{O}\rangle_{\mathrm{pq}}=\frac{\int dx\mathcal{O}(x)|e^{-S(x)}|}{\int dx|e^{-S(x)}|},\quad \theta=-i\ \mathrm{Im}S$$

We need exp(# V) MC configurations (Sign problem)

- **Sign problem appears in various quantum systems e.g. systems incl. fermions at finite μ**

$$\det D(\mu)=[\det D(-\mu^*)]^*\to\det D(\mu\neq 0,\in\mathcal{R})\in\mathbb{C}$$

  - **Finite density QCD, Hubbard model off half-filling, Finite density fermion systems with repulsive int., ….**

Miserable ?

A New Hope (a la SW Episode IV): Lefschetz thimbles

- **Lefschetz thimble method**
  Witten ('10), Cristoforetti+ (Aurora) ('12), Fujii+ ('13), Alexandru+ ('16).
  - **Complexify integral variables**
    $x \to z = x + iy$
  - **Flow eq. from a fixed point σ (thimble)**
    → Im(S)=const.

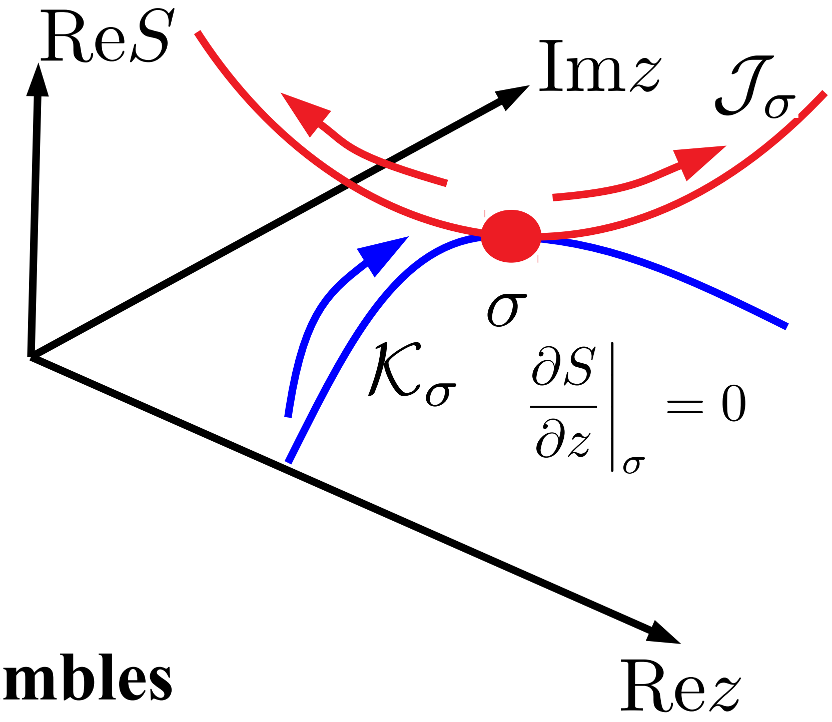
Thimble
https://muddyfaces.co.uk/

$$\mathcal{J}_\sigma : \frac{dz_i(t)}{dt} = \overline{\left(\frac{\partial S}{\partial z_i}\right)} \quad \text{(thimble)}$$

$$\to \frac{dS}{dt} = \sum_i \left|\frac{\partial S}{\partial z_i}\right|^2 \in \mathbb{R}$$

$$\int dx e^{-S} = \int_{\mathcal{C}} dz e^{-S}$$

$$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma \quad \text{(integral path)}$$

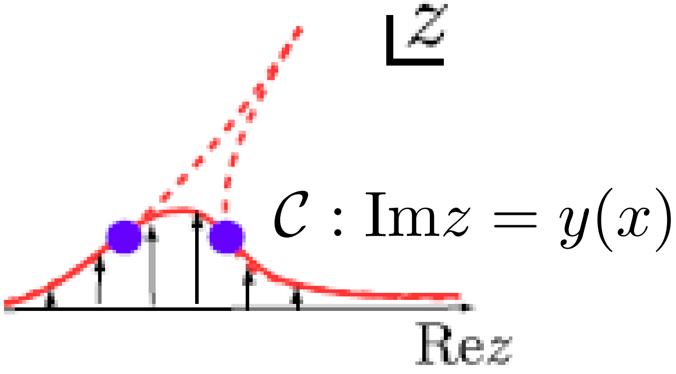


- **Problems:**
  Phase from measure and different thimbles

Path optimization method

- **Integral measure also has a phase.**

$$\mathcal{Z}=\int_{\mathcal{C}} dz e^{-S(z)}=\int dx J e^{-S(x+iy(x))}$$
$$=\int dx\left(1+\underline{i\frac{dy}{dx}}\right)\exp(-\mathrm{Re}S-\underline{i\mathrm{Im}S})$$



Path Optimization

- **Let us enhance the average phase factor by optimizing the path.**

$$\langle e^{i\theta}\rangle_{\mathrm{pq}}=\frac{\int dx J[y(x)]e^{-S(x+iy(x))}}{\int dx|J[y(x)]e^{-S(x+iy(x))}|}=\frac{\mathcal{Z}[y(x)]}{\mathcal{Z}_{\mathrm{pq}}[y(x)]}\begin{array}{l}\longleftarrow\textbf{path indep.}\\ \longleftarrow\textbf{path dep.}\end{array}$$

$$\mathrm{APF}=|\langle e^{i\theta}\rangle_{\mathrm{pq}}|$$

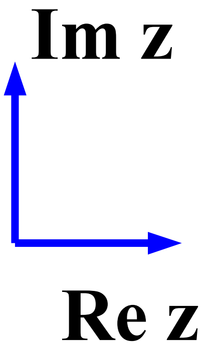
> ***Sign problem with complexified variables***
> ***~ Optimization problem of integration path***
> ***→ Neural network may work !***

Do neural networks help us to search for the path ?

$$\mathcal{Z} = \int dx(x+i\alpha)^p \exp(-x^2/2)$$

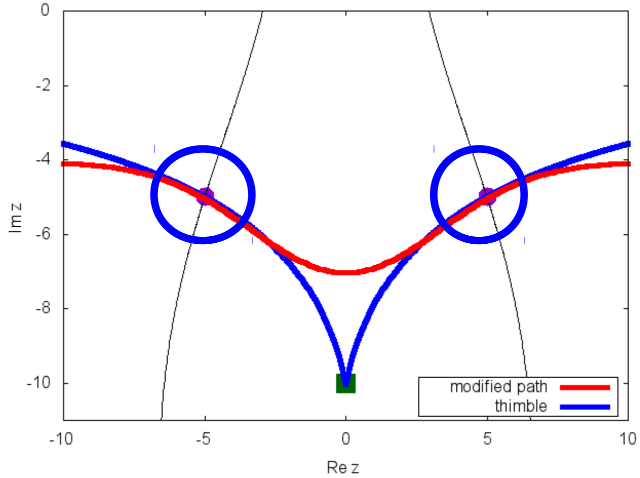
J. Nishimura, S. Shimasaki ('15)

Gaussian+Gradient Descent

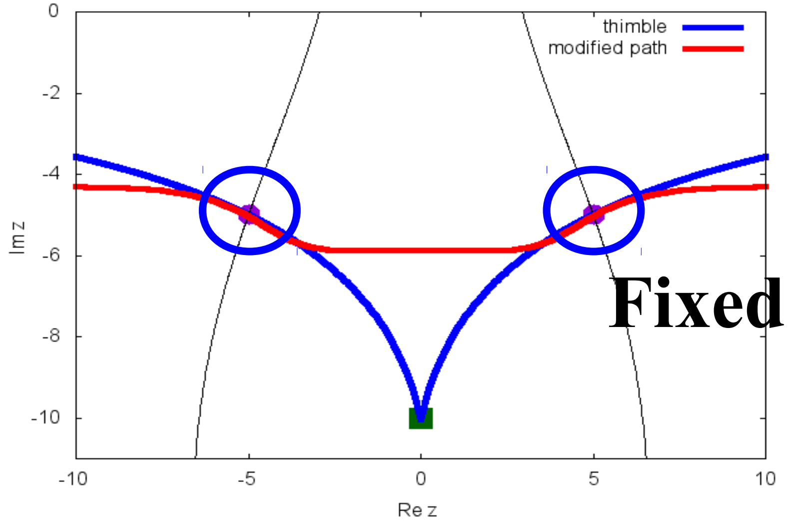


Im z

Re z

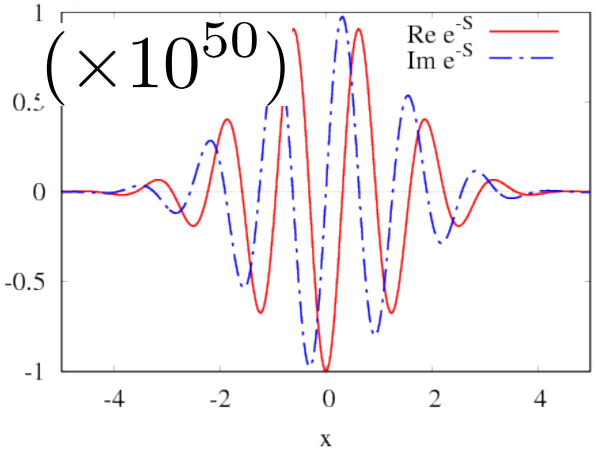


Neural Network

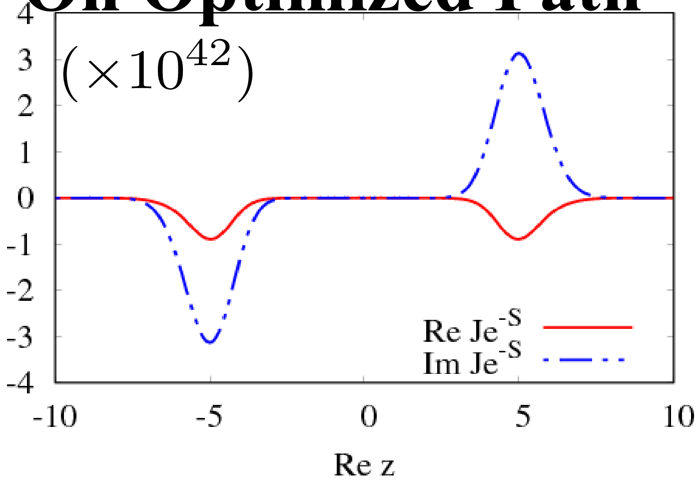


Fixed pt.

On Real Axis



On Optimized Path

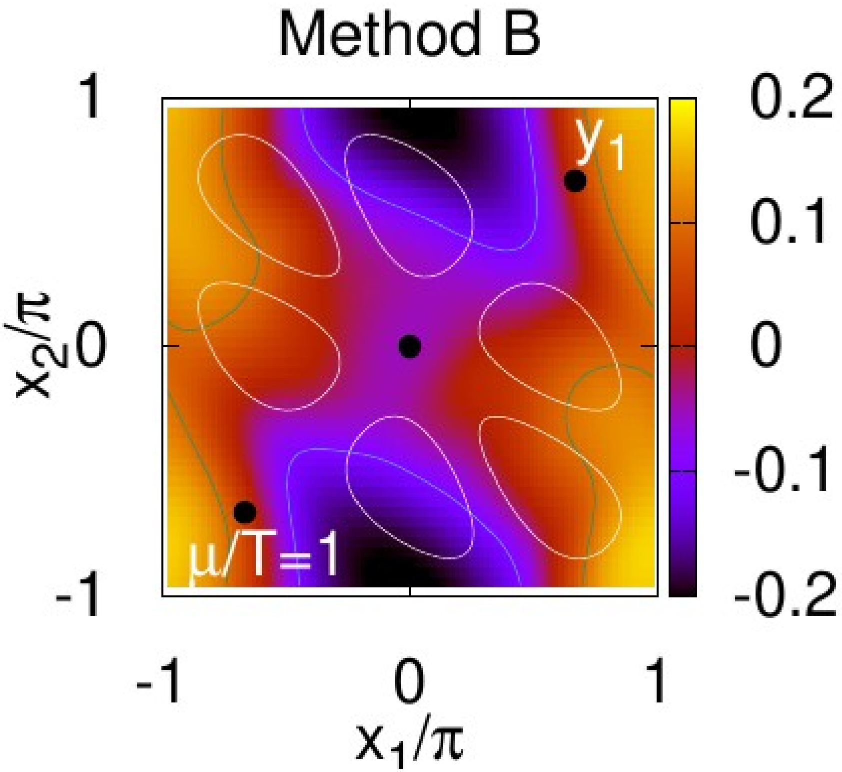


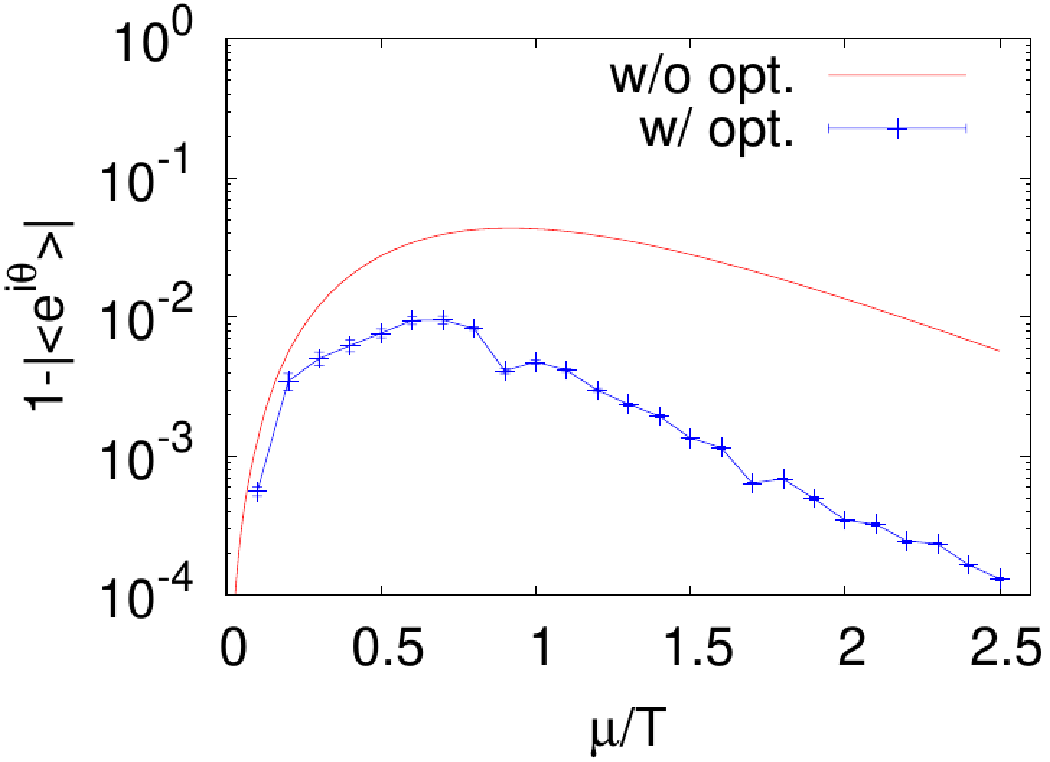
Mori, Kashiwa, AO ('17); AO, Mori, Kashiwa (Lat 2017)

Do neural networks help us to search for the path ?

- **0+1 dimensional lattice QCD at finite density**
  - **Complexification of link variables** $U \in \mathrm{SU}(3) \to \mathcal{U} = UH \in \mathrm{SL}(3)$
  - **Hybrid Monte-Carlo**

    Dynamical variable = U ∊ SU(3) , Hamiltonian = Re(S)
  - **Mono hidden layer neural network, Stochastic gradient method**





Mori, Kashiwa, AO, arXiv:1904.11140

Summary

- **Sign problem can be regarded as an optimization problem of the integral path in complexified variable space.**
- **Neural networks help us to search good integral path (manifold) (when the real axis is a reasonable initial state).**
  - **Any fn. can be reproduced at (hidden layer unit #) → ∞ (Universal approximation theorem)**
    G. Cybenko, MCSS 2 ('89) 303, K. Hornik, Neural networks 4('91) 251
- **The sign problem is still difficult to solve in realistic systems.**
  - **Two or more thimbles having different signs contribute to the partition fn.**
    → Tempered Lefschetz thimble ? ***Fukuma, Matsumoto, Umeda ('19)***
  - **Numerical cost of optimization with Jacobian effects $\propto$ O(V^3)**
    → Sparse Jacobian matrix approximation
    Alexandru+('18), Bursa, Kroyter ('18)
  - **Very complicated manifold → Deep learning ?**

Thank you !

Akira Ohnishi [1], **Yuto Mori** [2], **Kouji Kashiwa** [3]
1. Yukawa Inst. for Theoretical Physics, Kyoto U.,
2. Dept. Phys., Kyoto U., 3. Fukuoka Inst. Tech.

Y. Mori (PhD stu.)

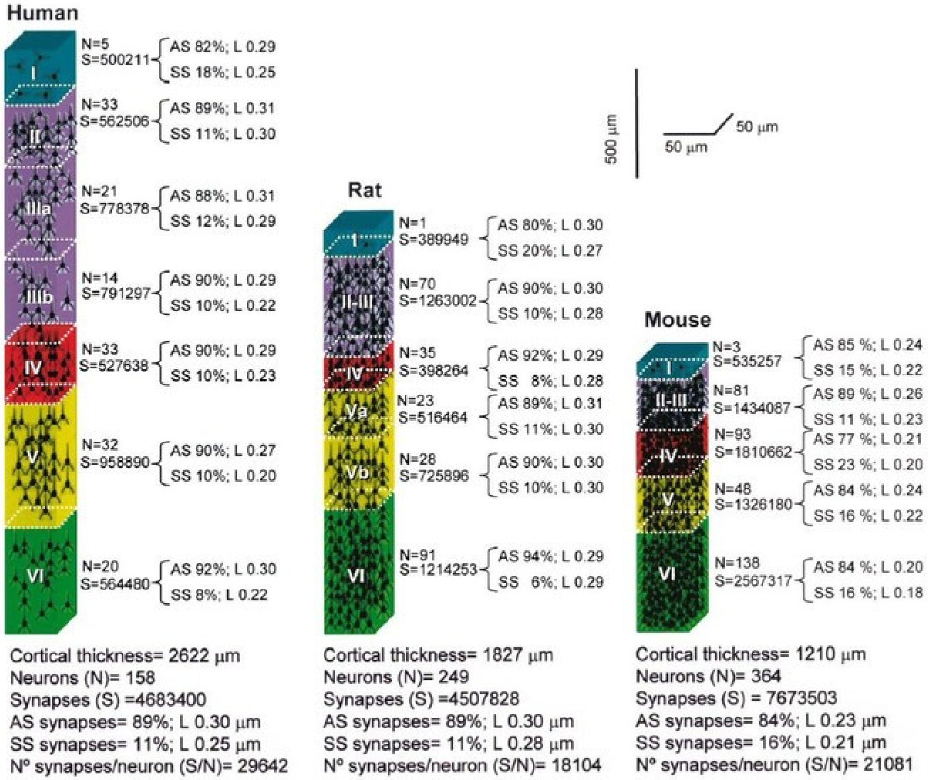
K. Kashiwa

AO (11 yrs ago)

- *1D integral: Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]*
- *φ^4 w/ NN: Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]*
- *Lat 2017: AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [arXiv:1712.01088]*
- *NJL thimble: Y. Mori, K. Kashiwa, AO, PLB 781('18),698 [arXiv:1705.03646]*
- *PNJL w/ NN: K. Kashiwa, Y. Mori, AO, PRD 99 ('19), 014033 [arXiv:1805.08940 [hep-ph]*
- *PNJL with vector int. using NN: K. Kashiwa, Y. Mori, AO, arXiv:1903.03679 [hep-lat]*
- *0+1D QCD: Y. Mori, K. Kashiwa, AO, 1904.11140; AO, Y. Mori, K. Kashiwa, arXiv:1812.11506 (Lat2018 proc.)*

Deep Learning

- **Deep learning (# of hidden layers > 3) may be helpful to explore complex paths, which human beings (~ 7 layers) cannot imagine, while "Understanding" the results of machine learning need to be done by human beings (at present).**



Defelipe 2011a (Review). The evolution of the brain, the human nature of cortical circuits, and intellectual creativity. Front Neuroanat 5, 29.

Euler-Lagrange equation for the integral path

- **Maximizing APF = Minimizing phase quenched partition fn.**

$$\mathcal{Z}_{\rm pq} = \int d^N\varphi_R \left| \det\left(\delta_{ij} + i\frac{\partial\varphi_{j,I}}{\partial\varphi_{i,R}}\right) \exp[-S(\varphi_R + i\varphi_I)] \right|$$

$$= \int d^N x \, |W(x_i + iy_i, \partial_i y_j)| \ \ (\varphi = x + iy(x))$$

- **Stationary condition of $\mathbf{Z_{pq}}$ w.r.t. y(x) → Euler-Lagrange eq.**

$$\frac{\delta}{\delta y_j}\mathcal{Z}_{\rm pq} = 0 \to \left[\frac{\partial}{\partial x_i}\frac{\partial}{\partial(\partial_i y_j)} - \frac{\partial}{\partial y_j}\right] |W(x+iy, \partial y)| = 0$$

- **One variable Euler-Lagrange equation**

$$\ddot{y} = (1+\dot{y}^2)^2 \left[\frac{\partial({\rm Im}S)}{\partial x} + \frac{\dot{y}}{1+\dot{y}^2}\frac{\partial({\rm Re}S)}{\partial x}\right] \quad (\dot{y} = dy/dx, \ddot{y} = d^2y/dx^2)$$

Example of repulsive vector-type interaction

- **One-Site Hubbard model (strong coupling limit → Hopping term=0)**

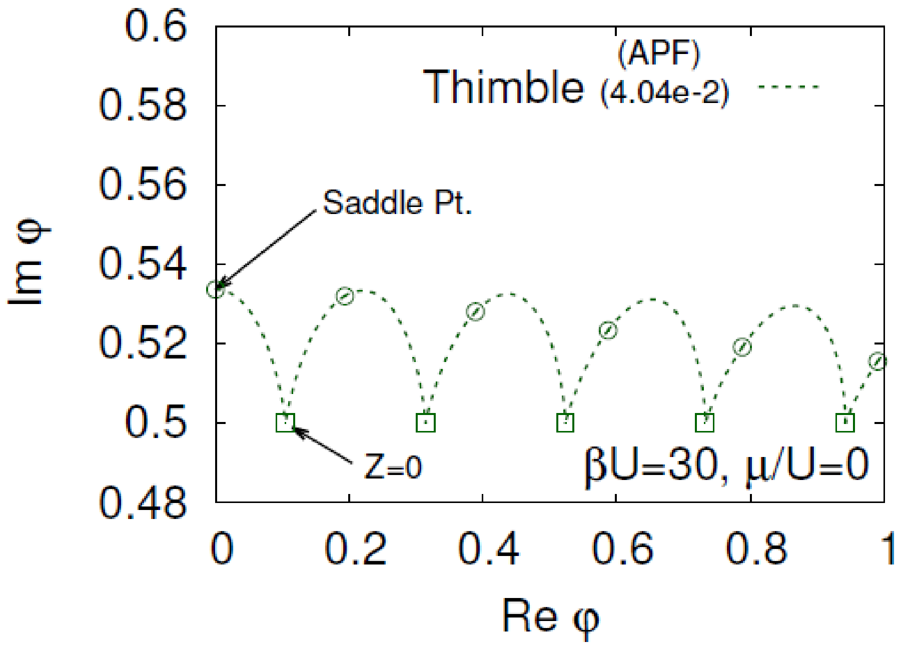
$$S = U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) \quad (n_i = \psi_i^\dagger \psi_i)$$

- **Path integral representation** *Tanizaki, Hidaka, Hayata ('16)*

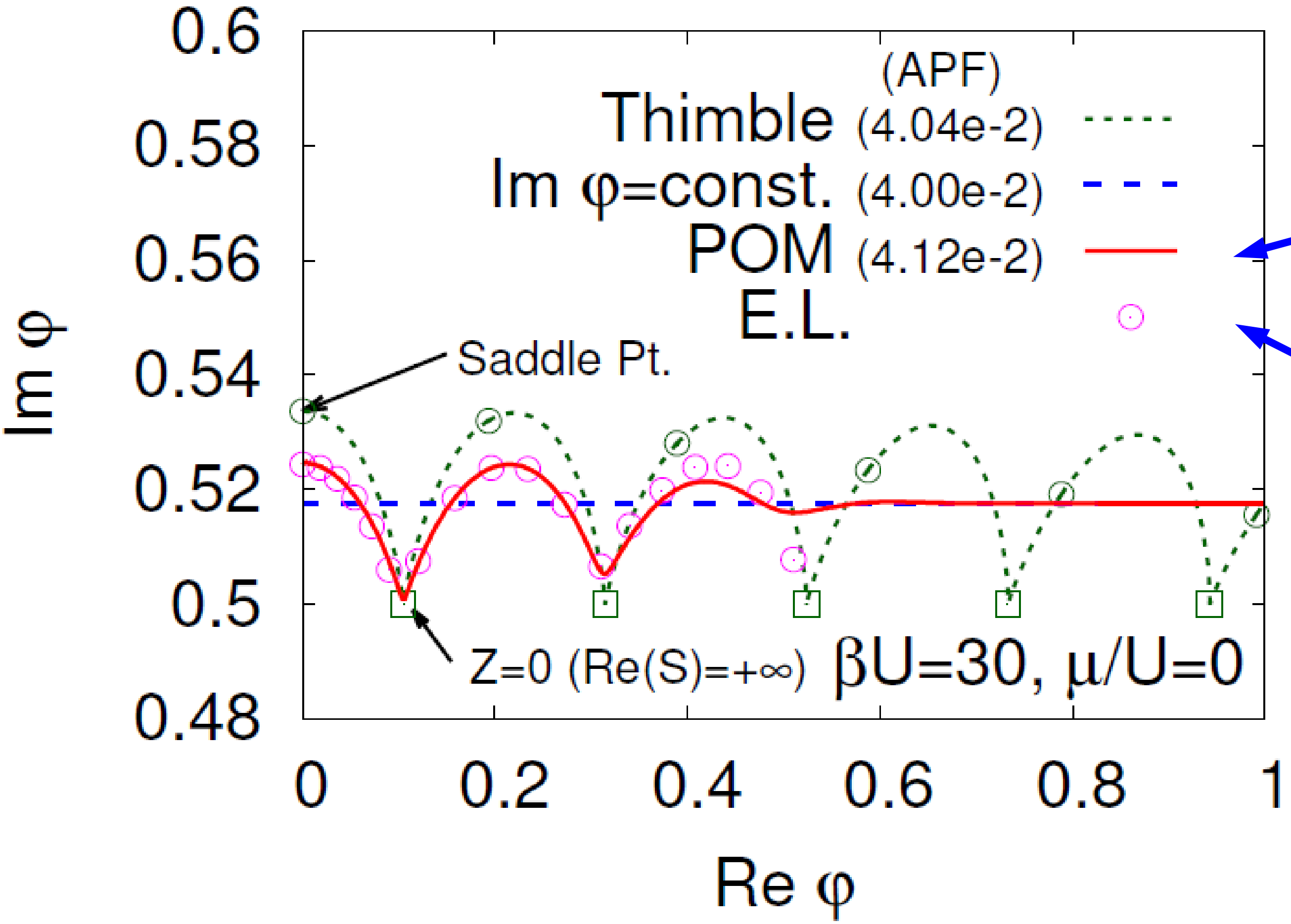
$$\mathcal{Z} = \sqrt{\frac{\beta U}{2\pi}} \int d\varphi \, [1 + \exp(\beta U(i\varphi + \mu/U + 1/2))]^2 \exp[-\beta U \varphi^2/2]$$

Complex !

- **Cancellation among multi-thimbles and # of thimbles increases with β = 1/T**



Example of repulsive vector-type interaction



Variational POM

Solution of EL eq.

POM works also in multi-thimble prb.

AO, Mori, Kashiwa, in prep.