矩阵：要求大概记内容，结构分类 → 12 大分解

特殊矩阵：对角阵.

$$\left\{\begin{array}{l} LU \\ QR \\ SVD \end{array}\right.$$

$$H = -\xi\sigma \quad , \quad \sigma = \pm 1$$

$\xi$ 无序 $\int p(\xi)\,d\xi = 1$

$$Z = e^{-\beta\xi} + e^{\beta\xi} = e^{-\beta F}$$

$$\Leftrightarrow F(\xi) = -\frac{1}{\beta}\ln\left(e^{-\beta\xi} + e^{\beta\xi}\right)$$

$$F = \langle F(\xi)\rangle = \int -\frac{1}{\beta}\ln\left(e^{-\beta\xi} + e^{\beta\xi}\right) p(\xi)\,d\xi$$

$$I = \int \ln\left(e^{-x} + e^{x}\right) e^{-\alpha x^2}\,dx$$

$$\underbrace{\text{Plot}[\,\text{NIntegrate}[\,\ln(e^{-x}+e^{x})\,e^{-\alpha x^2}, \{x, -100, 100\}]}_{\text{函数}},\{\alpha, 0.001, 10\}]$$

α给定

Plot NIntegrate 组合很有用

$\alpha \to \infty$ $\qquad \underline{\ln(e^{x}+e^{-x})}\, e^{-\alpha x^2}$

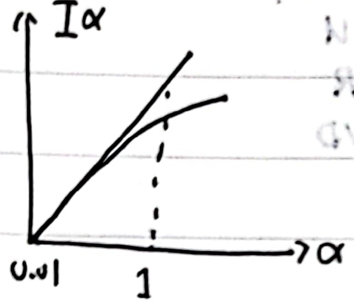
$x \to 0$

$$I = \int \ln\left(e^{x} + e^{-x}\right) e^{-\alpha x^2}\,dx$$

$$= \int \ln\left(2 + x^2\right) e^{-\alpha x^2}\,dx$$

$$= \int \left(\ln 2 + \frac{x^2}{2}\right) e^{-\alpha x^2}\,dx = \ln 2 \int e^{-\alpha x^2}\,dx = \ln 2\sqrt{\frac{\pi}{\alpha}}$$

$\alpha \to 0$.




猜测 $\alpha_0 = 1$

$\alpha_1 \sim \frac{\pi}{4}$ ; $\frac{\pi^2}{12}$

$$f(\alpha) = \alpha_0 + \alpha_1 \alpha + \alpha_2 \alpha^2 + \cdots$$

$\begin{cases} 1.0086 \\ 1.001 \\ 1.010 \end{cases}$ $\begin{cases} 0.786 \\ 0.81 \\ 0.805 \end{cases}$

$\alpha \to 0$, 如何做解析计算.

Mathematica 积不出.

$$\int dx \, (\ln(e^x + e^{-x}) - |x|) e^{-\alpha x^2} + \int dx \, |x| e^{-\alpha x^2}$$

$$2\int_0^{+\infty} (\ln(e^x + e^{-x}) - x) e^{-\alpha x^2} dx$$

$$\simeq 2\int_0^{+\infty} (\ln(e^x + e^{-x}) - x) dx$$

$$= 2\int_0^{+\infty} (\ln[e^x (1 + e^{-2x})] - x) dx$$

$$= 2\int_0^{+\infty} \ln(1 + e^{-2x}) dx.$$

$$\ln(1+x) = \sum (-1)^{n-1} \frac{x^n}{n}$$

$$= 2\int_0^{+\infty} \sum_n (-1)^{n-1} \frac{e^{-2nx}}{n} dx$$

$$= 2\sum \frac{(-1)^{n-1}}{n} \int_0^{+\infty} e^{-2nx} dx$$

$$= 2\sum_{n=1}^{+\infty} \frac{(-1)^n}{n} \frac{1}{2n} = \sum_{n=1}^{+\infty} \frac{(-1)^n}{n^2} = \frac{\pi^2}{12}$$

$e^{-\alpha x^2} = 1 - \alpha x^2 + \frac{\alpha^2}{2} x^4$

高阶

$\int_0^{+\infty} \ln(1+e^{-2x}) e^{-\alpha x^2} dx$

$= \sum_{n=1}^{+\infty} \frac{(-1)^{n-1}}{n} \int_0^{+\infty} e^{-2nx} (1 - \alpha x^2 + \frac{\alpha^2}{2} x^4 - \cdots) dx$

$\int_0^{+\infty} e^{-\alpha x^2} x^n dx = \frac{\alpha^{n-1}}{n!}$

总结：①数值分析

②拟合与猜测

③在数值下讨论.

物＝数＋模＋近似.

矩阵：三对角阵.
$O(N^2)$ 时间
$O(N)$ 内存.

$O(N^3) = O(N'^2)$　$N' = N^{\frac{3}{2}} \sim 10^6$

$N = 10^4$

Lanczos 方法. H. 构造三对角阵.

$A: n \times n$ matrix

目的：求A的本征值　$n > 10^6$

表示方式：
$\begin{cases} A v_n = \lambda_n v_n, \\ A|v_n\rangle = \lambda_n |v_n\rangle \end{cases}$　$v_n$: vector $= \begin{pmatrix} \vdots \end{pmatrix}$

算子＝矩阵

A已知，但不可能存储

Lanczos matrix.

由 $v$ 出发（态量与 $A$ 的本征态接近），归一化.

$$A v_1 = \alpha_1 v_1 + \beta_1 v_2 .$$

$$\begin{cases} v_1^+ \cdot v_2 = 0 \\ v_1^+ v_1 = 1 \\ v_2^+ v_2 = 1 \end{cases}$$

$$\begin{cases} v_1^+ A v_1 = \alpha_1 \\ v_2^+ A v_1 = \beta_1 \end{cases}$$

$$A v_2 = \gamma_1 v_1 + \alpha_2 v_2 + \beta_2 v_3 .$$

$$A v_n = \gamma_{n-1} v_{n-1} + \alpha_n v_n + \beta_n v_{n+1}$$

$\forall n \geq 2$. 只和 $v_{n-1}$、$v_n$ 正交，从而产生一个新的矢量 $v_{n+1}$.

$$\left[ A(\underbrace{v_1, v_2, v_3, \ldots, v_{N_c}}_{N\times N_c \text{ 的矩阵}}) \right]$$

类比： ~~A~~ $Hx = Ex$

$$\sum_j H_{ij} x_j = E x_i$$

$$\gamma_{n-1} v_{n-1} + \alpha_n v_n + \beta_n v_{n+1} = A v_n$$

$x_i \to v_i$

$E \to A$

$(\gamma_n, \alpha_n, \beta_n) \to H_{ij}$.

$$\Rightarrow \underbrace{\begin{pmatrix} \ddots & & & & \\ & \gamma_{n-2} & \alpha_{n-1} & \beta_{n-1} & \\ & & \gamma_{n-1} & \alpha_n & \beta_n \\ & & & \gamma_n & \alpha_{n+1} & \beta_{n+1} \\ & & & & & \ddots \end{pmatrix}}_{\text{三对角阵}} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = A \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}.$$

只需存 $\alpha_n \; \beta_n \; \gamma_{n-1}$.

求H的本征值 or 微分方程 ： 目标：能求 $\forall\, V(x,y)$ 的本征值.

$$\left\{ -\frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x) = E\psi(x)$$

离散化. $\psi(x) \Rightarrow \psi_i = \psi(x_i)$ $\left[ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E\psi(x)$

计算需要做矢量网化.

$$\psi'(x) = \lim_{h\to 0} \frac{\psi(x+h) - \psi(x)}{h}$$

$$-\frac{\partial^2}{\partial x^2}\psi(x_i) = \frac{\psi(x_{i+1}) + \psi(x_{i-1}) - 2\psi(x_i)}{h^2}$$

$$-\frac{1}{2h^2}(\psi_{i+1} + \psi_{i-1} - 2\psi_i) + V(x_i)\psi_i = E\psi_i$$

下一节课 $h \to 0$. $h \to 0$, 结果收敛.