High-dimensional Approximation

1. High-dimensional differential equations

1. The curse of dimensionality

Example: high-dimensional Poisson equation

\[ \begin{cases} -\Delta u = f \\ u = 0 \end{cases} \quad \text{on } \Omega = (0,1)^d \quad \text{and } \Omega \]

\[ \Delta \text{ is the Laplace operator, } \Delta u = \frac{\partial^2 u}{\partial x_1^2} + \ldots + \frac{\partial^2 u}{\partial x_d^2} \]

Suppose that solution \( u: \Omega \to \mathbb{R} \) is unique and \( u \in C^4(\Omega) \).
Discritization by finite differences:

Choose $N \in \mathbb{N}$, let $h = \frac{2}{N}$

Approximate solution at grid points:

$$x_n = (n_1 h, ..., n_d h) = nh$$

$$n = (n_1, ..., n_d) \in \mathbb{Z} \{0, ..., N \}^d \text{ multi-index}$$

Scale $u_n \approx u(x_n)$

Lemma: For every $v : \mathbb{R}^d \to \mathbb{R}$ with $v \in C^4$, we have

$$v''(x) = \frac{1}{h^2} (av(x-h) - 2v(x) + v(x+h)) + O(h^2)$$

Proof: Taylor expansion

Approximate

$$\frac{\partial^2 u(x_n)}{\partial x_{ij}^2} \approx \frac{1}{h^2} \left( u(x_n - he_j) + 2u(x_n) + u(x_n + he_j) \right) = \frac{1}{h^2} \left( u_{n-1} - 2u_n + u_{n+1} \right)$$

$e_j = (0, ..., 0, 1, 0, ..., 0)$

$i$-th entry

$\Rightarrow$ Solve the linear system

$$- \frac{1}{h^2} \sum_{j=1}^d \left( u_{n-i} - 2u_n + u_{n+i} \right) = f_i (x_n) \text{ if } n \in \{1, ..., N \}$$

$$u_n = 0 \text{ if } n_j = 0 \text{ or } n_j = N \text{ for some } j$$
This system can be written as
\[-Ly = b \text{ with } y \in \mathbb{R}^n, L \in \mathbb{R}^{n \times n}, b \in \mathbb{R}^n\]

**Example:** If \( n = 1 \), then \( y = (y_1, \ldots, y_{n-1})^T \),
\[b = (f(x_1), \ldots, f(x_n))^T\]
\[L = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}\]

The matrix \((-L)\) is symmetric and positive definite
\(\Rightarrow\) unique solution \((u_n)\)

**Accuracy:** \(\max_{x \in \mathbb{R}} |u(x) - u_n| \leq C h^2 \) if \( u \in C^2(\mathbb{R})\)

**Problem:** \( n = (N-1)^d \)

Computational work: at least \( O(n) \)
Memory: at least \( O(n) \)

**Examples:**
\[N = 10 \Rightarrow h = 0.1, \text{ error } \approx 10^{-2}\]
\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
d & 1 & 2 & 3 & 4 & 5 & 10 \\
\hline
n & 5 & 52 & 725 & 6561 & 55045 & 3.45 \times 10^5 \\
\hline
\end{array}
\]

\(N = 20 \Rightarrow h = 0.05, \text{ error } \approx \frac{1}{9} \times 10^{-2}\)
\[
\begin{array}{|c|c|c|c|c|c|}
\hline
d & 1 & 2 & 3 & 4 & 5 \\
\hline
n & 13 & 361 & 16855 & 130321 & 2476059 \\
\hline
\end{array}
\]
Consequences:

- Using twice as many grid points in each direction multiplies the computational work by $2^d$.
- Adding one more dimension to the problem does not mean adding some more work. It means that the work is multiplied by $(N-1)$.

Example: $N=100$, $d=2 \Rightarrow N = 10^6$, $d=4 \Rightarrow N = 10^8$

Example: Your life has $d=3$ and a weekly workload of $90$ h $\approx (3.92)^3$.

If our world was 4-dimensional, you would have to work

$(3.92)^4 \approx 136.9 \text{ h/week} \approx 13.6 \text{ h/day}$

(including weekends)

The fact that numerical work and memory requirements grow exponentially with respect to the dimension $d$ is called

\[ \text{THE CURSE OF DIMENSIONALITY} \]

(Bellman 1962)

Goal: Find approximations which avoid this. In this lecture, we study

- sparse grids
- wavelet compression
- variational approximations
2. High-dimensional differential equations

Why bother about $d > 3$?

(a) Quantum mechanics: Schrödinger's equation

Consider a molecule with $n$ particles (electrons or nuclei) moving in the three-dimensional space.

The state of the system is represented by the wave function

$$\psi : \mathbb{C}^n \times \mathbb{R}^{3n} \rightarrow \mathbb{C}$$

$$\psi = \psi(t, x_1, \ldots, x_n), \quad x_j \in \mathbb{R}^3$$

Normalisation:

$$\int_{\mathbb{R}^{3n}} |\psi(t, x)|^2 \, dx = 1 \quad \forall t \in \mathbb{C}$$

Interpretation: Let $\Omega = \Omega_1 \times \cdots \times \Omega_n$ with $\Omega_j \subset \mathbb{R}^3$. Then

$$\int_{\Omega} |\psi(t, x)|^2 \, dx \quad \text{is the probability that at time} \ t$$

the $j$-th particle is in $\Omega_j \quad (j = 1, \ldots, n)$.

Time-dependent Schrödinger equation:

$$i \hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_j} \Delta_j \psi + V \psi$$

Erwin Schrödinger 1926

$\hbar$: Planck's constant

$m_j$: Mass of the $j$-th particle

$\Delta_j$: Laplace operator w.r.t. $x_j$

$V(x)$: Potential (interaction between particles)
This is a differential equation in $e^{3t}$ dimensions (first order in time, second order in space).

Example: $\text{CO}_2$ (carbon dioxide) has 3 nuclei and 22 electrons

$\Rightarrow n = 25, \quad d = 75, \quad \gamma : \text{tend} \quad \Rightarrow \text{tend}$

Remark: $\text{CO}_2$ is still a rather small molecule...

\[ 20.14.03 \]

(6) Financial mathematics: Black-Scholes equation

Let $S(t)$ be the price of a stock at time $t$.

European call option:
At a fixed time lead, the holder of the option has the right to buy an underlying asset at the price $K$ from the seller of the option.

Example:
At time $t=0$, we buy 5 call options at the price $V_0$.
Each option gives us the right to buy 100 UMT shares at the price of $150 \text{€}$ each at time $t=\text{tend}$.
Suppose that at time $t=\text{tend}$, the stock exchange value of UMT is $100 \text{€}$ per share. If we exercise our option, we win

\[ 5 \times 100 \times (100 - 50) - 5 \times V_0 \]
If at time \( t \) the value of \( K/T \) is less than \( \text{the strike \$10} \),
then we do not exercise our option and lose \( V \).

**Question:** How can the value \( V(t, S) \) of an option be determined?

\[
V(t, S) = \begin{cases} 
S - K & \text{if } S \geq K \\
0 & \text{else}
\end{cases}
\]

Under a number of assumptions, \( V(t, S) \) solves the

**Black-Scholes equation**

\[
\frac{\partial V}{\partial t} = -\frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} - rS \frac{\partial V}{\partial S} + rV \\
V(t, S) = \begin{cases} 
S - K & \text{if } S \geq K \\
0 & \text{else}
\end{cases}
\]

where:
- \( S \) is the share price,
- \( K \) is the strike price,
- \( r \) is the risk-free interest rate,
- \( \sigma \) is the volatility of the share,
- \( t \) is the time until expiration.

**Fischer Black & Myron Scholes 1973, Robert C. Merton 1973**

**Nobel Prize 1997**

Consider how a basket option with \( d \) underlying assets.

\( \Rightarrow \) \( d \)-dimensional Black-Scholes equation

\[
\frac{\partial V}{\partial t} = -\frac{1}{2} \sum_{i=1}^{d} \sigma_i^2 S_i^2 \frac{\partial^2 V}{\partial S_i^2} - \sum_{i=1}^{d} S_i \frac{\partial V}{\partial S_i} + rV
\]

\( d \)-dimensional PDE, first order in time, second order in space.
Consider a reaction system with species $S_1, ..., S_d$ and $m$ reactions:

$$
S_1 + S_2 \rightarrow S_3 \\
S_3 \rightarrow S_1 + S_2 \\
S_4 + S_5 \rightarrow S_4 + S_4
$$

Each of the species is a set of indistinguishable particles with the same properties.
Each particle moves and interacts randomly with other particles.

Applications: chemical reaction systems, gene regulatory networks, spread of contagious diseases in a population, ...

Goal: Compute the probability $p(t, n)$ that at time $t$ there are exactly $n_i \in \mathbb{N}_0$ particles of $S_i$ ($i = 1, ..., d$).

**Chemical Master Equation**

$$
\frac{\partial p(t, n)}{\partial t} = \sum_{j=1}^{m} \left( \gamma_j (n - y_j) p(t, n - y_j) - \gamma_j (n) p(t, n) \right)
$$

$\gamma_j (n) \in \mathbb{R}$: propensity of the $j$-th reaction

$y_j \in \mathbb{R}^d$: stoichiometric vector of the $j$-th reaction

$\Psi : \mathbb{N}_0^d \rightarrow \mathbb{R}$: initial distribution
Examples:

\[ S_1 + S_2 \rightarrow S_3 \quad \alpha(n) = c_1, n_1, n_2 \quad \Lambda_1 = \binom{1}{2} \binom{3}{2} \]
\[ S_3 \rightarrow S_1 + S_2 \quad \alpha(n) = c_2, n_3 \quad \Lambda_2 = \binom{1}{2} \binom{3}{2} \]

(CHE) \equiv \text{set of ODEs, "discrete PDE"}

Problem: Have to compute p(t,n) for all n \in \mathbb{N} \rightarrow \text{inhom. problem!}

Transition: Compute p(t,n) only for all n \in \{0, ..., N-1\}^d

\implies \text{Tell Nth unknowns!}

\text{Curse of dimensionality}

Traditional methods fail.

(a) Fokker–Planck equations

Let \( f: \mathbb{R}^d \rightarrow \mathbb{R}^d \), \( g: \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m} \) \((d, m \in \mathbb{N})\)

Consider the stochastic differential equation (SDE)

\[ dx(t) = f(X(t)) dt + g(X(t)) dW(t) \]

\( X(t) \in \mathbb{R}^d \) random variable, \( W(t) \) standard Wiener process

Interpretation: ODE + noise term

\[ \frac{dX(t)}{dt} = f(X(t)) + g(X(t)) \frac{dW(t)}{dt} \]

\( \overbrace{\text{ODE}}^{\text{ODE}} \) \( \overbrace{\text{noise term}}^{\text{noise term}} \)
Let $g(t,x)$ be the probability density of $X(t)$, i.e.

$$
P(X(t) \in \Omega) = \int \limits_{\Omega} g(t,x) \, dx,
$$

and let $g(0,x) = g_0(x)$ be given. Then $g(t,x)$ satisfies the Fokker-Planck equation

$$
\begin{cases}
\frac{\partial g}{\partial t} + \sum_{j=1}^{d} \frac{\partial}{\partial x_j} (F_j(x) g(t,x)) + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j} (G_{i,j}(x) g(t,x)) = 0 \\
g(0,x) = g_0(x)
\end{cases}
$$

where $G(x) = G(x) \delta^2(x) \in \mathbb{R}^{d \times d}$

$$
G_{i,j}(x) = \sum_{i=1}^{n} g_{i,j} \delta^2(x)
$$

$d$-dimensional PDE, first order in time, second order in space.