Solving differential equations with neural networks, October 21, 2024

Solving differential equations with deep neural networks

$$\frac{dg}{dx} = -\gamma g(x)$$

$$x \in [0, \infty)$$

$$g(x) = g_0 \exp(-\gamma x)$$

$$g_0 = g(x=0)$$

Population growth

$$\frac{dg}{dt} = \alpha g(t)(A - g(t))$$

$\alpha > 0$, growth rate $A > 0$ max population

$g(0) = g_0$

analytical solution:

$$g(t) = \frac{A g_0}{g_0 + (A - g_0)(\exp(-\alpha A t))}$$

Exponential decay

$$\frac{dg}{dx} - (-r g(x)) = 0$$

$$= f(x, g(x), g'(x)) = 0$$

In general

$$f(x, g(x), g'(x), g''(x) \ldots g^{(n)}(x)) = 0$$

Finite difference schemes

Taylor expand

$$g(t+\Delta t) = g(t) + \Delta t \cdot \frac{dg}{dt}\Big|_t + \frac{(\Delta t)^2}{2!} \frac{d^2 g}{dt^2}\Big|_t + O(\Delta t^3)$$

Discretize $t \to t_i$

$t_i = t_0 + i\Delta t \quad i = 0, 1, 2, \ldots n$

$t_n = t_0 + n\Delta t \Rightarrow$

$$\Delta t = \frac{t_n - t_0}{n}$$

$$g(t+\Delta t) \to g(t_i + \Delta t) = g_{i+1}$$

$$g_{i+1} \simeq g_i + \Delta t \, g_i'$$

$$\left.\frac{dg}{dt}\right|_{t=t_i} = g_i'$$

start $i = 0$

$$\frac{dg}{dt} = -\gamma g(t)$$

$$g_1 \simeq g_0 - \gamma g_0$$

$$-\gamma g(t=0)$$

$$= -\gamma g_0$$

$$g_2 \simeq g_1 - \gamma g_1$$

$$\vdots$$

$$g_n \simeq g_{n-1} - \gamma g_{n-1}$$

$$\varepsilon(\Delta t^2)$$

Two-point boundary value

$$-g''(x) = f(x) \quad \text{known function}$$

$x \in [0, 1]$

$g(x=0) = g(x=1) = 0$

(Dirichlet boundary condition)

$$f(x) = (3x + x^2)\exp(x)$$

$$g(x) = x(1-x)\exp(x)$$

$$g''(x) = \frac{g(x+\Delta x) + g(x-\Delta x) - 2g(x)}{(\Delta x)^2}$$

$$+ \; o(\Delta x^2)$$

$$-g''(x) \simeq -\frac{\left(g(x+\Delta x) + g(x-\Delta x) - 2g(x)\right)}{\Delta x^2}$$

$$= f(x)$$

$$x \to x_i = x_0 + i\Delta x$$

$$i = 0, 1, \ldots, n \qquad \Delta x = \frac{x_n - x_0}{n}$$

$$-g_i'' = -\frac{d^2 g}{dx^2}\Big|_{x = x_i}$$

$$-g_i'' = \frac{-g_{i+1} - g_{i-1} + 2g_i}{\Delta x^2} = f_i$$

$$\Rightarrow \quad Ag = \Delta x^2 f$$

$$g = \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_{n-1} \end{bmatrix} \qquad g_0 = g_n = 0$$

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Neural Networks

$$f\left(x, g(x), g'(x), \ldots, g^{(n)}(x)\right) = 0$$

Trial solution

$$g_t(x) = h_1(x) + h_2(x, N(x, \theta))$$

satisfies initial and/or Boundary conditions

Exponential decay

$$g_t(x) = g_0 + x N(x, \theta)$$

Two-point boundary value

$$g_t(x) = x(1-x)\,N(x, \in)$$

$$x=0 \qquad g_t(0) = 0$$

$$x=1 \qquad g_t(1) = 0$$

Define cost function

$$C(x, \in) = \frac{1}{n}\sum_{i=0}^{n-1}\left(f\left(x_i, g_t(x_i), g_t'(x_i), \ldots g_t^{(m)}(x_i)\right)\right)^2$$

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_i \left[f(x_i, g_t(x_i, \theta), g_t'(x_i, \theta), \dots g_t^{(m)}(x_i, \theta)) \right]^2$$

exponential decay

$$C(x, \theta) = \frac{1}{n} \sum_i \left(g_t'(x_i, \theta) - (-\gamma g_t(x_i, \theta)) \right)^2$$