Physics-Informed Neural Networks (PINNs) for Grain Drying Problem

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What is drying process ?

Defintion

Drying is a mass transfer process consisting of the removal of water or another solvent by evaporation from a solid, semi-solid or liquid.

Drying applications

The drying process can help lower costs of transportation and storage by removing unnecessary liquid volume in a material. It is used in :

1. Food science and vegetables
2. Industry (e.g., drying wood)
3. Pharmacy (e.g., drying vaccines)
4. Agriculture (e.g., grain drying)

Grain Drying Process !

Grain drying is the process of drying grain to prevent spoilage during storage.
It can be modeled by a couple (or not) between :

1. The heat transfer equation
2. The mass transfer equation.

Numerical methods

The grain drying process is numerically solved using the following approach :

1. Finite difference method ;
2. Finite element method ;
3. Volume element method ;

Disadvantages

However these methods present some disadvantages :

1. Meshing almost impossible for complex study areas ;
2. Discretization too difficult for high dimensional PDEs ;
3. Stability study ;
4. Consistency study ;
5. ...

Towards Scientific Machine Learning (SciML) !

1. SciML is multidisciplinary and draws on expertise from applied and computational mathematics, computer science, and physical laws.
2. It is a data-driven scientific discovery method that relies on machine learning and scientific computing tools.
3. PINNs is one example.

Benefits

1. Use of a deep neural network ;
2. Collection of a large amount of data (Big Data) ;
3. Regularity of the approaching solution ;
4. Automatic differentiation (e.g., Backpropagation)
5. Free mesh

Thinking about the project !

This project relies on/involves :

1. agricultural research engineering (e.g., Grain drying process),
2. and applied mathematics problem (e.g., PDEs).

Research question

The main research question of this thesis is the following :

How can we approach the grain drying problem, together with associated storage, with scientific machine learning (SciML), in particular PINNs ?

Underlying abstract grain drying process

To develop such a novel PINNs-based model for grain drying, it is necessary to have a fundamental understanding of :

1. Type of grain (e.g, peanut, maize, rice, soya beans, coffee) ;
2. Grain's geometry (e.g, cylindrical) ;
3. Drying method (e.g, solar drying, hot-air drying) ;
4. Type of storage (e.g., Deep-bed Dryer) ;
5. Heat and Mass transfert equations between grain and air ;
6. Parameters affecting drying process.

Research Objectives

The main research objectives of this thesis are listed below :

1. Choose of a grain which should be relevant in Africa (Modeling).
2. Implement PINNs for this problem.
3. Convergence analysis for PINNs.
4. Real world application

Contribution

1. Motivation : No PINNS-based grain drying
2. Contribution to future research in drying applications
3. Comprehensive theoretical and computational investigations of PINNs

Initial Research Project (Mathematical model)

Below is the system of semilinear parabolic equations to describe the grain drying process :

$$
\begin{cases}
\rho_a C_{pa}\left(\epsilon \dfrac{\partial T_a}{\partial t} + V_x \dfrac{\partial T_a}{\partial x}\right) - \dfrac{\partial}{\partial x}\left(\lambda_a \dfrac{\partial T_a}{\partial x}\right) - h_1(T_g - T_a) - h_2(T_L - T_a) \; = \; 0 \\
\rho_g C_{pg}(1-\epsilon)\dfrac{\partial T_g}{\partial t} - \dfrac{\partial}{\partial x}\left(\lambda_g \dfrac{\partial T_g}{\partial x}\right) - h_1(T_a - T_g) - h_3(T_L - T_g) \\
\qquad -h_4\alpha\left(W - \dfrac{M}{\Gamma(T_g)}\right) - w(T_g) \; = \; 0 \\
\epsilon \dfrac{\partial W}{\partial t} + V_x \dfrac{\partial W}{\partial x} - \dfrac{\partial}{\partial x}\left(D_W(T_a)\dfrac{\partial W}{\partial x}\right) + \alpha\left(W - \dfrac{M}{\Gamma(T_g)}\right) \; = \; 0, \qquad 0 < x < L, \\
\dfrac{\partial M(x,r,t)}{\partial t} - \dfrac{D_M(T_g)}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial M}{\partial r}\right) \; = \; 0, \qquad 0 < r < R, \; 0 < t < t_f
\end{cases}
\tag{1}
$$

Initial Research Project (Variables)

where :

1. T_a is the air temperature,
2. T_g is the grain temperature,
3. W is the air humidity,
4. M is the grain moisture content,
5. α is the grain surface,
6. h_j are heat transfer coefficients,
7. C_{pg} and C_{pa} are the specific heat of grain and air,
8. ρ_g and ρ_a are the specific mass of grain and air,
9. ε is the porosity,
10. V_x is the air velocity,
11. $w(T_g)$ is the biological heat,
12. D_W and D_M are diffusivities.

The system (1) is equipped with the following initial conditions :

$$\begin{cases} T_a(x,0) - T_a(x) &= 0, \\ T_g(x,0) - T_g(x) &= 0, \\ W(x,0) - W(x) &= 0, \\ M(x,r,0) - M(x,r) &= 0, \end{cases} \tag{2}$$

and boundary conditions :

Initial Research Project (Boundary conditions)

$$
\begin{cases}
T_a(0,t) - T_0 = 0, \\
\lambda_a \dfrac{\partial T_a}{\partial x} - k(T_L - T_a(L,t)) = 0, \\
-\lambda_g \dfrac{\partial T_g}{\partial x} - k(T_0 - T_g(0,t)) = 0, \\
\lambda_g \dfrac{\partial T_g}{\partial x} - k(T_L - T_g(L,t)) = 0, \\
W(0,t) - W(T_0) = 0, \\
D_W(T_a)\dfrac{\partial W}{\partial x} - \nu(W(T_L) - W(L,t)) = 0, \\
r^2 \dfrac{\partial M}{\partial r} = 0, \\
D_M(T_g) R^2 \dfrac{\partial M}{\partial r} - \mu\left(W - \dfrac{M(x,R,t)}{\Gamma(T_g)}\right) = 0,
\end{cases}
\tag{3}
$$

Problem Description

Problem :

We consider the Boundary Initial Value Problem (BIVP) : Find the unknown function $u = [T_a, T_g, W, M]$ such that the systems $(1) - (3)$ are satisfied.

The main aim is to approximate the classical solution u of this problem with PINNs.

Before we proceed, let us introduce the residuals R_{pde}, R_{ini} and R_{bou} by :

$$\begin{cases} R_{pde}[u](x,r,t) = D_1(x,t) + D_2(x,r,t) + D_3(x,t) + D_4(x,t) \\ R_{ini}[u](x,r,0) = I_1(x,0) + I_2(x,r,0) + I_3(x,0) + I_4(x,0) \\ R_{bou}[u](x,r,t) = [B_1 + B_2](x,t) + [B_3 + B_4](x,t) \\ \qquad + [B_5 + B_6](x,t) + [B_7 + B_8](x,r,t) \end{cases} \tag{4}$$

PINNs approach (step2)

where

1. $\{D_i\}$ represents the four equations in order in the system (1),
2. $\{I_i\}$ represents the four equations in order in the system (2),
3. and $\{B_i\}$ represents the eight equations in order in the system (3).

Using these residuals, one measures how well a function u satisfies our BIVP. Note that the exact solution u_e will satisfy :

$$R_{pde}[u_e] = R_{ini}[u_e] = R_{bou}[u_e] = 0. \tag{5}$$

PINNs approach (step3)

Our goal is to approximate the solution u of our BIVP with deep neural networks u_θ, where θ represents the neural network's parameters. To this end, we have the following minimization problem :

$$\min_{\theta} L(\theta) \;=\; \left\| R_{pde}[u_\theta](x,r,t) \right\|_2^2 + \left\| R_{ini}[u_\theta](x,r,0) \right\|_2^2 + \left\| R_{bou}[u_\theta](x,r,t) \right\|_2^2 \quad (6)$$

This formula (6) is called the generalization error. It involves integrals (due to the L_2-norm) and can therefore not be directly minimized in practice.

PINNs approach (step4)

Since the training is done on these sampling points $\left\{\{(x_s, r_s, t_s)\}_{i=1}^{N_s}\right\}$ for $s = i, j, k$, equation (6) is replaced by the empirical loss function (e.g., training error) :

$$\min_{\theta} L(\theta) = \sum_{i=1}^{N_i} \left|R_{pde}[u_\theta](x_i, r_i, t_i)\right|^2 + \sum_{j=1}^{N_j}\left|R_{ini}[u_\theta](x_j, r_j, 0)\right|^2$$
$$+ \sum_{k=1}^{N_k}\left|R_{bou}[u_\theta](x_k, r_k, t_k)\right|^2 (7)$$

Schematic diagram of PINNs

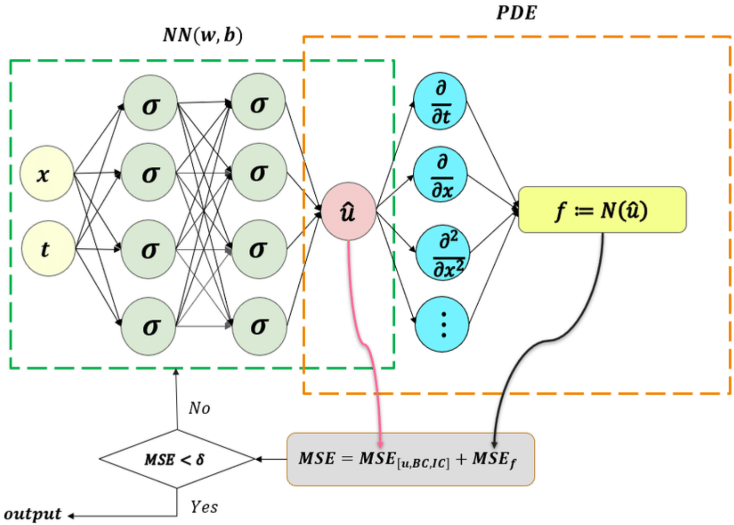

Figure:

Expected results

1. A model that can be interpreted with a level of confidence.
2. Obtain certifiable methods i.e., we want to be able to stick a label on the solution saying that it is going to be accurate for all reasonable inputs.
3. Good agreement with the experiment.

Further works

1. Sampling methods (e.g., numerical integration)
2. Approximation theory
3. Data-driven Loss function
4. Optimisation (by using ML tools)

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End

Thanks for listening !