Permafrost Modeling using Physics Informed Neural Networks (PINNs)

The Natural Disasters: Yeonwoo Jeon, Ajeet Subramanian, Michael Zhou

Github: https://github.com/ajeet-sub/SciML-Permafrost-Modeling

Abstract

To model permafrost distributions in earth's cryosphere, many models are composed of a simulation derived with the 1-dimensional heat equation as a governing equation. To better project the effects of climate change, models have shifted to using the 1D heat conduction equation with phase change to better account for the variabilities in thermodynamics present in many permafrost grounds currently. While these models provide accurate results, they primarily do this through a discretization of the governing equation, using the centered finite difference method, which is often computationally expensive. For our project we aim to integrate a scientific machine learning approach that can reduce the run times of modeling the mean annual ground temperature (MAGT) and active layer thicknesses of permafrost sites by at least 20%, while maintaining a high accuracy. In our approach, we integrate a physics informed neural network (PINN) with loss functions physically constrained by the 1D heat conduction equation as well as its boundary/initial conditions. We compared this approach to 3 other scIML approaches that could be considered and discussed their pros and cons, while also discussing some expected results for our design. With this paper, we hope to introduce a scientific machine learning framework that could be applied and help improve the field of permafrost modeling.

Motivation

Permafrost regions are one of Earth's most important carbon reservoirs. Large amounts of greenhouse gasses including carbon dioxide and methane will be released from sequestered organic materials as permafrost thaws. Predicting thaw patterns or analogously the future extent of permafrost is essential for anticipating these trends and future climate scenarios. Another aspect of warming permafrost is how it will destabilize the land about important infrastructure to local communities. Warming permafrost causes soil compaction that will change Arctic and sub-Arctic landscapes. The impact of permafrost thawing can change over decades, so there is a need for robust models that can reliably predict their changes even into the far future [1].

Problem Characteristics

Traditional models commonly have limitations in capturing complex interactions, especially in contexts of feedback loops between soil temperature and moisture. We aim to incorporate physics-informed ML models to create more robust simulations for these interactions. In addition, observational data in remote areas for permafrost regions are very sparse. Incorporating both limited observational and simulated data can help generalize predictions, which can potentially be scaled to accommodate for live data feed in the future. Embedding physical models into ML comes with additional benefits as the model can be more sensitive to changes in variables like soil moisture and temperature.

Prior Work

The established methods for permafrost modeling involve two main categories or types of models: empirical-statistical models and process-based models. Empirical-statistical models generally work by relating permafrost occurrences and characteristics directly with topo-climatic factors. At times criticized for being gray boxes, they see use for being easy to use and requiring limited input parameters as well as being relatively reliable if well calibrated locally or regionally [5]. The new popularity of machine learning approaches has inevitably brought such applications to permafrost, resulting in models that would fall into this category of model where the underlying process is not directly involved but approximated using data.

As far as recent attempts at using machine learning for this problem, one example is a study done on the Seward Peninsula, Alaska by Thaler et al. The study achieved accuracies between 70%- 90% using classifiers using random forest, support vector machines, and neural networks. Satellite data was used to predict permafrost trends [2]. There was also a study done on the Qinghai-Tibet Plateau (QTP) area, utilizing ensemble ML models to evaluate the factors influencing thermokarst lake formation, which form due to permafrost thaw [3]. Finally, a study is present using physically informed systems, training on the integrated dataset from observations with the heat equation as a constraint. They were able to achieve RMSE down to 0.5C, compared to 1.5C from the Kudryavtsev model [4].

In contrast to empirical-statistical models, process-based models more explicitly describe the heat flow between the surface and the permafrost and the propagation of that energy into the ground. They are suited for sensitivity studies with respect to interactions and feedbacks involved under climate-change scenarios where the steady-state assumptions of simpler models fail to capture [10]. The allure of using a more physics-informed machine learning model is the hope that we will be able to achieve performances and granularity of results that matches the results of these more intense process-based models with less compute compared to the computationally expensive numerical solvers usually used for these models.

Two process-based models we investigated as possible inspirations and benchmarks we wanted to compare our approach to were the Cryogrid models and GIPL 2.0. At a fundamental level, both models use a simple enthalpy model to model the energy flux at the boundary between the ground surface and the air temperature while using a form of the heat equation to describe the distribution of the subsurface temperatures [12-13]. Aside from the surface air temperature, which acts as a forcing term, these models take into consideration numerous other parameters such as the liquid water content of the soil as well as multiple soil parameters for each layer of the soil. Some examples of these soil parameters include the soil porosity and thermal conductivity. For more accurate modeling of winter months, snow depth and the snow density is used to determine how much the snow will act as a buffer to trapping summer heat in the ground and moderating the chilling effect of the colder winter temperatures. Both models achieve very high accuracies for fine-grained predictions and modeling when properly calibrated to a region's numerous parameters. Both use standard numerical methods like Centered Finite Difference (for GIPL 2.0) to perform the forward simulation of the underlying PDE.

GIPL 2.0 was the benchmark decided to be the benchmark we will compare against due to its simpler nature as well as the fact that it was built for use in Alaska in particular, and through Global Terrestrial Network for Permafrost (GTNP) database there is a lot of Alaskan ground temperature data publicly available [11]. Cryogrid was not used as a benchmark since it was developed primarily with mountain regions in mind, which results in a need for very fine spatial precision in snow modeling and many other bells and whistles to account for large differences in altitude over small distances [10].

Approaches Considered

Physics-Informed Neural Network (PINNs)[6]

PINNs integrate neural networks with governing physical equations, making them ideal for scenarios with sparse observational data. They directly incorporate the 1D heat conduction equation into the loss function, allowing the model to adhere to physical principles even with limited data. This method aligns with our goal to reduce computational expense while maintaining accuracy and was selected as our primary approach.

Deep Data Assimilation (DDA)[7]

DDA combines traditional data assimilation techniques with neural networks to refine predictions over time. DDA requires large amounts of high-quality data and is computationally expensive. While useful for systems with lots of data, its limitations make it less suitable for our problem, which relies heavily on sparse datasets from boreholes.

AI Feynman Symbolic Regression[8]

Symbolic regression is great at generating interpretable models for nonlinear features and potential future uses (especially if done by hand). However, it is not designed for direct simulation of output variables and generation of interpretable models itself is not the focal point of our project. We want to be able to create a model that inherits scientific information into outputting meaningful values, not necessarily obtaining an interpretable representation of it.

Multiple Physics Pretraining (MPP) for Surrogate Models[9]

MPP excels at combining multiple independent physical equations into a unified model. This is especially effective if the equations are coming from different domains that are independently crucial in output values. However, the simplicity of our system governed simply by the 1D enthalpy equation makes it excessive.

Our Approach

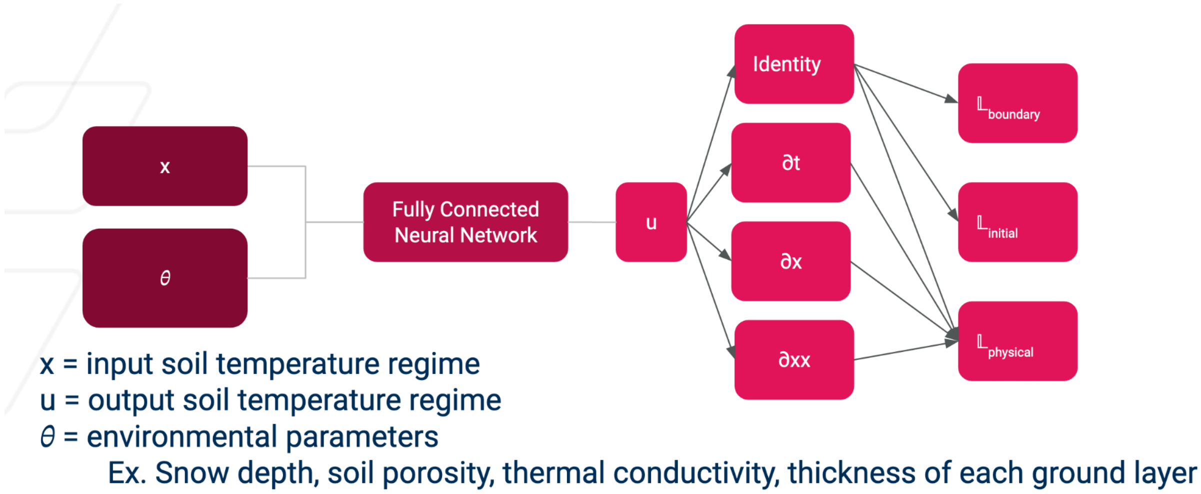

Figure 1. Model Architecture

Our choice of model is the Physics-Informed Neural Network (PINN) as the main framework for our modeling. The PINN model will inherit the 1D heat conduction equation into its loss functions given some of our borehole sensor data as its boundary conditions. The approach is expected to be effective especially considering the sparse nature of our observational data. Our approach will leverage a few following aspects:

For loss functions using the 1D heat conduction equation, the boundary conditions and initial conditions are discretized from the original continuous version of the equation. Following are the said continuous versions of the loss terms that will be discretized before implementation.

$$\mathbf{L}_{total} = \mathbf{L}_{RMSE} + \mathbf{L}_{physical} + \mathbf{L}_{boundary} + \mathbf{L}_{initial}$$

- $\mathbf{L}_{physical} = \mathbf{L}_{time} - \mathbf{L}_{spatial} \quad where:$

$$\mathbf{L}_{time} = \frac{\partial H}{\partial t} = c(x, T) \cdot \frac{\partial \widehat{T}}{\partial t} + L(x) \cdot \frac{\partial \omega}{\partial t}$$

$$\mathbf{L}_{spatial} = \nabla \cdot (k \nabla \widehat{T}) = \frac{\partial}{\partial x} \cdot \left(k \frac{\partial \widehat{T}}{\partial x} \right)$$

- $\mathbf{L}_{boundary} = \mathbf{L}^{surface}_{boundary} + \mathbf{L}^{bottom}_{boundary} \quad where:$

$$\mathbf{L}^{surface}_{boundary} = \widehat{T}(x_{surface}, t_{initial}) - T(x_{surface}, t_{initial})$$
$$\mathbf{L}^{bottom}_{boundary} = k\frac{\partial \widehat{T}}{\partial x} + q_{geothermal}$$

- $\mathbf{L}_{initial} = \widehat{T}(x, t_{initial}) - T(x, t_{initial})$

When discretized along with squared values to allow minimization combined with hyperparameters λ to adjust each weights, the above total loss term becomes:

$$\mathbf{L}_{total} = \lambda_{MSE}\mathbf{L}_{MSE} + \lambda_{physical}\mathbf{L}^{2}_{physical} + \lambda_{boundary}\mathbf{L}^{2}_{boundary} + \lambda_{initial}\mathbf{L}^{2}_{initial}$$

- $\mathbf{L}_{physical} = \mathbf{L}_{time} - \mathbf{L}_{spatial} \quad where:$

$$\mathbf{L}_{time} = c(x, \widehat{T}) \cdot \frac{\widehat{T}(x,t_{i+1}) - \widehat{T}(x,t_i)}{\Delta t_i} + L(x) \cdot \frac{\omega(x,t_{i+1}) - \omega(x,t_i)}{\Delta t_i}$$
$$\mathbf{L}_{spatial} = k \cdot \frac{\left(\widehat{T}(x_{i+1}, t_i) - \widehat{T}(x_i, t_i)\right) - \left(\widehat{T}(x_i, t_i) - \widehat{T}(x_{i-1}, t_i)\right)}{(\Delta x_i)^2} = k \cdot \frac{\widehat{T}(x_{i+1}, t_i) - 2\widehat{T}(x_i, t_i) + \widehat{T}(x_{i-1}, t_i)}{(\Delta x_i)^2}$$

- $\mathbf{L}_{boundary} = \mathbf{L}^{surface}_{boundary} + \mathbf{L}^{bottom}_{boundary} \quad where:$

$$\mathbf{L}^{surface}_{boundary} = \widehat{T}(x_{surface}, t_{initial}) - T(x_{surface}, t_{initial})$$
$$\mathbf{L}^{bottom}_{boundary} = k \cdot \frac{\widehat{T}(x_{bottom}, t_{any}) - \widehat{T}(x_{1\,from\,bottom}, t_{any})}{x_{1\,from\,bottom} - x_{bottom}} + q_{geothermal}$$

- $\mathbf{L}_{initial} = \widehat{T}(x_i, t_0) - T(x_i, t_0)$

Experiments/Baseline Model

For our baseline comparison, we are planning on comparing the performance of our PINN to that of the GIPL 2.0 model detailed in the prior works section. Our primary reasoning for this choice is its strength particularly in predicting the permafrost distributions in the Alaska region, which is where we'll be acquiring our observational data for both training and testing from. This model has been calibrated using observational data from Alaska, making it a well established benchmark for evaluating our model performance. GIPL 2.0 employs a numerical transient model based on the 1D heat conduction equation shown above. They also combine other environmental factors such as vegetation depth, snow depth, soil composition, and water content. Usage of a centered finite difference method for solving these equations shows high accuracy but seems to have high computation requirements in contrast.

By comparing the PINN approach to GIPL 2.0, we aim to address two key aspects:

1. Computational efficiency: The GIPL 2.0 model is known for its high computational demand especially with its finite difference discretization method. With their resolution and amount of parameters, computation is expensive. The PINN

framework in contrast can combine physical constraints with machine learning, potentially reducing the computational overhead.

2. Predictive performance: While the GIPL 2.0 model has shown robust predictive performance in the past with the Alaska region, it depends heavily on environmental data especially for parameterization. PINNs are known to be able to work with sparse datasets effectively by embedding the governing physical laws directly into the learning process.

For comparison, we aim to evaluate the performances with a few metrics:

- Accuracy metrics: Statistical measures such as Root Mean Square Error (RMSE) and R^2 will be used to compare results to the observed data. This will show how well each model predicts permafrost properties such as Mean Annual Ground Temperatures and Active Layer Thickness.
- Computational efficiency: Mainly runtime will be measured for both training PINNs and evaluating GIPL 2.0. These values will be utilized to determine the relative performance and thus computational cost especially given other accuracy metrics at similar run times. The primary aim is to either be faster, or be more accurate if it takes more.

Expected Results

For our expected results, we hope to have plots and numerical results which answer the two facets of our model performance that we're looking to tackle with our research question: accuracy and computational efficiency.

To measure accuracy, we will compare the MAGT/ALT values of the GIPL model and the PINN and check their error by comparing it with observational data. Our main metric of measurement for this will be the root mean-squared error (RMSE) and R^2. Once we do this, we will compare the 2 results by looking at both their numerical values for the RMSE, but also adding some data visualizations to see if there are any trends in the values given by the models.

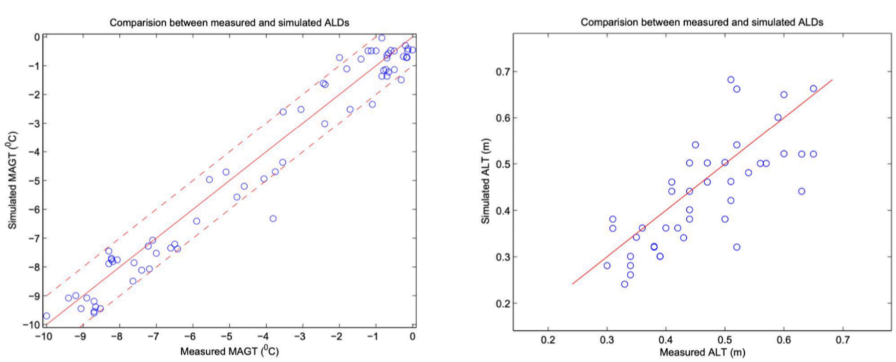

Figure 2. Measured vs Simulated values for the GIPL 2.0 model [12]

It is expected that with the PINN, the values for the MAGT and ALT will be close to that of the GIPL 2.0 baseline, resembling the plots shown above. Ideally, the values for the RMSE should either be around equal or lower than that of the baseline, showing the initial signs of how a scientific machine learning approach can improve evaluation performance in permafrost modeling.

To measure computational efficiency, we will compare the run times of the PINN and GIPL models to see which one runs faster. For the PINN, we will measure how long it takes to train the data and make predictions on the test data and have that as the run time. For GIPL, the run time will be the amount of time it takes for the simulation to start and finish. We expect the run time for the PINN to be much shorter compared to the GIPL model, as the numerical discretization is computationally expensive [12].

Risks and Model Limitations

We expect there to be potential issues and limitations that should be considered at minimum. While PINNs are designed to work with limited data, noisy data can result in poor generalization or overfitting given some boundary conditions. In our case, GTNP borehole datasets had an alarming number of missing values or NaNs. Oftentimes the GTNP borehole datasets would show “seasons” of data collection where certain features are prioritized over the other in an alternating fashion. Our attempt to mitigate this issue is to simply replace the NaNs with linearly interpolated data, but this cannot be a long-term solution and should be addressed in potential future developments of this project whether via actual data collection or other types of modeling process.

In addition, we expect the hyperparameters (especially the weights for each of the loss terms) to behave sensitively. The performance will highly depend on the combination of each loss term corresponding to physical, boundary, and initial conditions. Considering there is one for each term, a proper convergence will be time consuming. The weights will be searched on a small grid basis, with it allowing for larger gridspace provided additional computational power.

Potential Future Expansion

PINNs are known to have increasing difficulty especially with increasing number of layers. Because we are only implementing a single governing equation into relevant physical loss terms, PINNs remain relevant as a proof of concept and demonstration of Scientific Machine Learning application for Permafrost modeling. In the future, we expect expansions could be possible using models such as PiratesNet with specialization for additional architectural complexity (mainly additional layers), or MPP in case additional physical models could be accounted for.

If additional physical models were to be considered, one of the candidates could be the second law of thermodynamics, incorporating entropy balance into the system. This would allow the model to account for the amount of available work that can be extracted from a given system. Considering that properties for water are very well known, incorporating the second law of thermodynamics could potentially come in useful in permafrost modeling.

Conclusion

Our project demonstrates the potential application of Physics-Informed Neural Networks as a viable method compared to the traditional numerical methods for modeling permafrost. This is achieved by embedding the 1D heat conduction equation as loss terms, where the models then can estimate both Mean Annual Ground Temperature and Active Layer Thickness while adhering to physical thermodynamic properties. Our approach is particularly ideal for situations with sparse observational data, as it combines physical laws into the system.

We expect our results to show definite advantages of PINNs which is their ability to significantly reduce computational overhead while achieving similar performance. By achieving this, PINNs can be a viable solution for scalable permafrost simulators.

In the future, potential transfer to models such as PiratesNet or MPPs given proper thermodynamic contexts can be ideal for better performance. Specifically, PiratesNet can be ideal given sufficient data and computational power, since a deeper neural network could be utilized for more complex interactions. We also expect that additional data collection might come in handy especially with increased quality, consistency, and regional diversity. One of the main concerns with permafrost modeling in general is that each of the locations have slightly different profiles due to the local geography, and including methods to potentially account for local geography and diversity can be valuable.

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