A Physics-Constrained Neural Differential Equation for Data-Driven Seasonal Snowpack Forecasting

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ABSTRACT: This paper presents a physics-constrained neural differential equation for modeling seasonal snow depth (or density), given atmospheric conditions and the snow water equivalent, as a function of time. When trained on data from multiple SNOTEL sites, the model can predict daily snow depth timeseries with $\sim 9\%$ error on average and with Nash Sutcliffe Efficiencies of over 0.94 across a wide variety of snow climates, an improvement of more than 20% compared with established snow models. The model also generalizes to new sites not seen during training. Requiring the model to predict snow water equivalent as well as snow depth, as a fully standalone model, increases the error to $\sim 15\%$. The structure of the model guarantees respect of certain physical constraints and allows snow modeling at different temporal and spatial resolutions without additional retraining of the model. It can be easily incorporated into existing snow models as an additional prognostic equation, and holds potential for use in climate modeling as well as in water resource management or ecological research. We anticipate that the same model design can extend to other dynamical systems with physical constraints.
1. Rationale

Seasonal snowpacks serve a critical role in determining Earth’s climate, regulating Earth’s energy balance, and buffering storage of freshwater. They hold economic as well as ecological significance, as seasonal snow provides a majority of the United States’ water supply and over a sixth of the world’s supply, and plays a large role in agricultural, flood, drought, and avalanche risks (De Michele et al. 2013a; Gao et al. 2021). However, snowpacks are in turn susceptible to the climate state, and their long-term status is dependent on how the Earth’s climate changes in the future. Therefore, snowpack modeling and monitoring is important to carry out on both seasonal and multi-decadal timescales.

Modeling the evolution of seasonal snow for climate applications offers a challenging problem of scales; it is the bulk properties of the snow (albedo, snow cover fraction, snow temperature, and snow water content) that are critical, yet microphysical and location-specific processes dictate these properties and must be taken into account. The most detailed models output vertically-resolved snowpacks, including liquid percolation, phase changes, metamorphic effects, and other types of compaction; they are often calibrated and used on the site-level (e.g., De Michele et al. (2013b)). The simpler models used in climate simulations range in complexity from single-layer/bulk models to multi-layer models with parameterizations for one more bulk properties that are calibrated from observational data (e.g., Menard et al. (2021)). While the laws of physics ultimately govern the evolution of these snow properties, the computational requirements or uncertainty surrounding essential small-scale processes and their closures necessitate reduced parameterizations to permit detailed larger- or global-scale forecasts (Kapnick et al. 2018; Bair et al. 2018). Further uncertainties are exacerbated by data availability (Menard et al. 2021; Kouki et al. 2022).

The snow water equivalent, SWE, is typically used as a prognostic variable in bulk snow models, representing total water storage in the global water cycle and mass balance equations. It is related to the snow depth $z$ via the bulk snow density $\rho_{\text{snow}}$ and the density of liquid water $\rho_{\text{water}}$ as

$$\rho_{\text{water}} \cdot \text{SWE} = \rho_{\text{snow}} \cdot z.$$  \hspace{1cm} (1)

The density $\rho_{\text{snow}}$ affects the thermal, mechanical, and optical properties of snow at large and small scales, as well as mass/energy fluxes and a snowpack’s ability to hold melted water (Kouki et al. 2022).
The depth $z$ influences radiative absorption/emission, in turn affecting springtime thaw and the snowpack energy balance. To forecast seasonal snowpacks, an explicit model or observational data from sensors or satellite streams are required for at least two of the three quantities (SWE, $z$, and $\rho_{\text{snow}}$) that respect required energy and mass conservation laws as well as other physical limits on their evolution. However, for a given SWE, the snow depth and bulk density can vary considerably over time at a single location, or between locations under similar forcings, due to compaction, melting/refreezing cycles, and changes in the density of falling snow. The representation of these processes is where many of the challenges in snow modeling arises.

### a. Current Approaches

The majority of prevalent snow models follow a mixed approach between fully physical and empirical modeling, with parameterization for one or more of SWE, $z$, and $\rho_{\text{snow}}$. For instance, the Community Land Model (CLM5.0) empirically parameterizes new snow density and snow compaction rates in the update of $z$, which is combined with polynomial parameterizations for determining water fluxes in the update of SWE to approximate $\rho_{\text{snow}} = (\text{SWE}/z)\rho_{\text{water}}$ (Lawrence et al. 2019). The SNOWPACK model uses an entirely empirical model for snow density (Menard et al. 2021; Lehning et al. 2002). By contrast, the iSobal model takes snow depth data and a parameterized physics model for $\rho_{\text{snow}}$ to achieve an estimate for SWE (Hedrick et al. 2018). Such contemporary models and several proposed machine learning models (e.g., Bair et al. (2018); Meloche et al. (2022)) have led to satisfactory forecasting of northern hemisphere snowpacks, though they frequently result in total snow depth or SWE depth errors of over 15% when tested, especially beyond their training or calibration locations (Meloche et al. 2022; Ebner et al. 2021; Viallon-Galinier et al. 2020). Furthermore, it is unclear how well these models generalize to snowpacks in different climates, either in new locations or in a warmer world. A further drawback of empirical models is their statistical or black-box nature, which precludes interpretability. Additionally, they may not inherently respect conservation laws, impeding their capability to integrate into larger hydrology models (De Michele et al. 2013a; Gao et al. 2021).

Compared to empirical parameterizations, physical and process-based models aim to represent the evolution of snow in a manner that should (1) generalize to any snowpack (out-of-sample usage), (2) easily integrate into larger hydrology models and physical conservation laws for energy
and water, and (3) offer straightforward interpretation. However, unresolved small-scale processes create a real-world departure from idealized physics models that frequently require a large degree of complexity in multiple snow layers to faithfully recreate observed macroscopic properties. This leads to large computational overhead and makes such models unsuitable for inclusion in global models, despite the necessity of small-scale accuracy in accumulated global effects. The trade-offs between robustness, computational complexity, and resolution continue to challenge the snow modeling community and large-scale climate modeling.

b. Our contribution

The goal of this work is to investigate how observational data can be used to augment or replace physically motivated parameterizations for bulk snow depth (or snow density) for global climate simulations and seasonal forecasting. We use observational data from many locations to inform a model that can be applied at any location. The proposed model follows a hybrid approach between physically-based and empirical modeling in that it captures physical processes and is guaranteed to obey physical constraints, in a manner that is both computationally simple and easily incorporated into larger-scale hydrology models. Such an approach offers many of the benefits of both types of modeling while achieving similar and improved performance relative to existing models. The mathematical design and modularity of the model, based on learning a prognostic equation for snowpack height, also makes it easy to integrate within an existing hydrology model.

In a broader context, the proposed model demonstrates a general method for enforcing (or learning) hard threshold constraints of arbitrary functional form on the output of an optimizable data-driven model without augmentation of the loss function. The study of enforcing hard constraints via network structure remains a growing field of research (Jiang et al. 2019; Dong and Ni 2021; Beucler et al. 2021). The straightforward method we employ has applications in contemporary climate modeling as well as in other physics-emulating models that guarantees respect of conservation laws.
2. Methodology

a. Overview

We model the snowpack height $z$ at any given location by the ordinary differential equation

$$\frac{dz}{dt} = M(z, \text{SWE}, \varphi, R, v, T_{\text{air}}, P_{\text{snow}}),$$  \hspace{1cm} (2)

where $M$ is a neural network whose output is the rate of change in snowpack height (units of m s$^{-1}$), SWE is the snow-water equivalent (m), $\varphi$ is the relative humidity (between 0 and 1), $R$ is the broadband solar radiative energy flux (W m$^{-2}$), $v$ is the wind speed (m s$^{-1}$), $T_{\text{air}}$ is the air temperature ($^\circ$C), and $P_{\text{snow}}$ is the liquid water-equivalent rate of snowfall (m s$^{-1}$). Location and time dependencies are only indirectly encoded in the model through the choice of input variables (all are evaluated at the same instantaneous time and location), which allows the same model to be applied at different locations and with different temporal/spatial resolution, which we initially choose to be consistent with the frequency of the inputs. The model $M$ is empirical, but the goal of training is that it will learn to represent universal physical processes that apply independent of time and location. The model $M$ is generally nonlinear, but it encompasses linear models as well. Using a feed-forward neural network which only depends on the current state of the system makes this model easy to implement into existing land-surface models, since this is consistent with the differential equations being solved for other variables. By contrast, recurrent neural networks model $z$ directly, and require retaining a history of the state.

The predictor variables were selected using prior knowledge about their role in snowpack evolution and based on their widespread availability. All selected variables showed a correlation coefficient to the target variable $dz/dt$ equal to or above the conventional statistical significance threshold of $\approx 5\%$, validating their inclusion in the model.

Choosing to predict $z$ using SWE instead of predicting $\rho_{\text{snow}}$ or vice versa was determined by current capabilities to offer the most value and utility to contemporary climate modeling techniques (however, the model choice is simultaneously adaptable to alternative use-cases or when SWE is not available, see sections 2b and 3d). Globally distributed datasets of SWE observations are more prevalent than those of $z$ or $\rho_{\text{snow}}$, which broadens this model’s applicability. Within climate models, SWE is already explicitly calculated and tracked using conservation laws for water. Improving
predictions given SWE is equivalent to improving the prediction of bulk density via Eq. (1). With improved snow densities, snowpack properties such as thermal conductivity and liquid-water holding capacity can be more accurately estimated.

b. Predictive Model Structure

The model $M$ consists of two components. The first is a “predictive” component with trainable weights, used for generating a prediction of $dz/dt$. The second component of the network structure is a set of pre-determined functions with non-trainable weights, which enforce physical constraints on the prediction from the first component. The predictive network structure is shown in Fig. 1.

![Fig. 1. Structure of the predictive portion of the network. All blue lines indicate a trainable linear transformation of the input (of $k$ variables), including a bias. Colors indicate the activation function used upon collection at the node, as noted in the legend. The hyperparameter $n$ determines the width of the internal mixing layer.](image)

The architecture of the predictive network was chosen with the intent of remaining as simple as possible while maintaining performance, resulting in the choice of only two hidden layers, followed by a dense collapsing layer without an activation to the predicted value. As the number of collapsed features is the same as the number of inputs, the network could also be interpreted as a dense network with one hidden layer to transform the input variables in a nonlinear manner to system-relevant features, followed by a regression on those features. The width of this mixing layer is determined by the hyperparameter $n$ multiplying the number of input features $k$. This structure
is easily adaptable to a different choice or number of input features for additional case studies or alternative target predictions.

c. Model Constraints

The remainder of the network exists to impose explicit and hard constraints on the overall prediction. Specifically, any threshold constraints can be explicitly enforced in an absolute manner with a max/min function fixed to the output of the network. This is immediately realizable with the anonymous function capabilities of most contemporary automatic differentiation and network packages, but can still be realized for legacy systems or specialized constructions through direct fixing of additional dense layers containing ReLu activation on top of any predictive model, where ReLu is the Rectified Linear Unit (for a breakdown of the process, see Appendix a). Our model constraints will be presented through such dense layers for maximal convenience of implementation under any system.

1) Threshold Constraints for Snowpack Prediction

Constraints for snowpack height evolution $dz/dt$ should keep the snowpack depth rate of change within physical limits, with the goal of creating better generalizability as well as more stable behavior when the entire trained model $M$ is integrated over time. The constraints implemented for this specific application are as follows:

- Enforce non-negativity of snowpack height within a time step of length $\Delta t$, $M \geq -z/\Delta t$,
- Enforce the inability of $z$ to increase without snowfall, $P_{\text{snow}} = 0 \implies M \leq 0$. In principle, processes like wind drift can violate this constraint, but these affects are assumed to be minimal given the training data, see section 2d.

These constraints can both be represented as upper and lower threshold functions, the lower as $f_- = -z/\Delta t$ and the upper as $f_+ = \text{ReLu}(p) \times 1_{P_{\text{snow}} > 0}$, where $p$ is the output of the predictive portion of the network and ReLu is the Rectified Linear Unit. In this case, $z$, $P_{\text{snow}}$, $\Delta t$ are all nonnegative, meaning $f_-$ is nonpositive and $f_+$ is nonnegative, with $f_+ \geq f_-$ (the equivalence case when $z = 0$ and $P_{\text{snow}} = 0$). These properties simplify the computational requirements to enforce the constraints when enacted as a sequence of ReLu layers (see Appendix a), resulting in a final structure for $M$ as depicted in Fig. 2. Though the chosen constraint for this setup includes the
Fig. 2. Architecture of $M$, highlighting the constraint component attached to the predictive structure from Fig 1. The chosen structure enforces growth only under precipitation and non-negativity of snowpack height, and is equivalent to a max/min block on the output. Weight colors indicate the constant’s sign and activation functions follow the color scheme given in Fig. 1.

time step $\Delta t$, this does not explicitly impact the time dependency nor the resolution of the model. The predictive portion of the network contains no time nor time-step dependence, and its structure does not change after training. Choosing or changing $\Delta t$ appropriately scales the constraint, which permits its use in adaptive time-step schemes. This does not impact what values the predictive portion will output, only the physics-dictated minimum value that will be produced. In this manner the model is standalone, requiring only one round of training at one resolution to be used at any resolutions. It does not require additional control flow during use to maintain snowpack positivity when the scaling constant is adequately set—this reflects an inherent time-step independence that should not lead to significant time-step dependent effects when trained properly. The model is still limited by the temporal resolution of any input data. The only precaution is to train the model with data where the spread of calculated lower boundary values in the training data is mostly less than the expected spread of anticipated target values $dz/dt$ during post-training usage. Alternatively, choosing a constraint form without $\Delta t$ for employment under a different use-case also results in timestep independence.

2) Benefits of Structurally-Enforced Thresholding

The capability of a simple thresholding function affixed to a predictive model is sufficiently modular to enable many different types of constraint construction(s) $f$ on a predictive model $p$ (or
even learned constraints, see Appendix a) with minimal overhead cost and no loss of runtime or
resource complexity. It is impossible for a model with such thresholding to generate an output that
lies beyond the threshold(s) dictated by $f$. In the two-sided threshold case, an upper threshold $f_+$
and a lower threshold $f_-$, the model $M$ can then be interpreted as a function which interpolates
between two prescribed boundaries (e.g., a black-box model to predict drag between turbulent
and viscous limits), or that describes departures from a prescribed boundary in the one-sided
case. This facilitates integration into larger models obeying constraints from physical laws or
control flow (even when determined from non-predictive inputs) without breaking conservation
laws. The versatility of this approach provides utility for any predictive system where complex
processes cannot be analytically modeled in a comprehensive manner but hard limiting cases or
envelopes are theoretically provable. Hard boundaries also increase stability under an accumulated
time-stepping setting since outputs remain realistic, and the enforcement of these boundaries
during training enables gradients and subsequent weight updates to better predict values within
the boundaries, especially when augmented with soft constraints from data filtering and/or penalty
functions.

d. Data

For training, we used data from 37 sites in the United States Snow Telemetry (SNOTEL) network.
We selected the sites based upon simultaneous availability of $z$, SWE, $\varphi$, $R$, $v$, $T_{air}$, and precipitation
data between hourly and daily time series of their entire reporting histories. We used averaged
hourly data to fill missing values in reported daily time series and excised all sensor days without
daily or hourly data. Among individual time series, entire sensor calendar years were discarded
if a sensor showed sustained behavior of defective/unphysical measurements during that year
(which were otherwise individually excised) to avoid the assumptions and selection biases of more
sophisticated outlier methods, as the volume of available data at daily resolution was sufficient
for such choices. The incremental changes in height $\Delta z$, water content $\Delta$SWE, and time between
resulting measurements $\Delta t$ were evaluated. All data points with $\Delta t > 1$ day were excised, so that
the predicted quantity, or target, is $dz/dt \approx \Delta z/\Delta t$ for a given sensor day reporting start-of-day
$z$, SWE, day-averaged $\varphi$, $R$, $v$, $T_{air}$, and total daily precipitation. This resulted in 103854 usable
data points, spanning a wide variety of climates (Fig 3), which will improve the model’s ability to
generalize to different climates.

Fig. 3. Distribution of SNOTEL sites used for training the network. (a) Training sites as visualized over the
United States. (b) Training sites visualized with elevation vs their average nonzero snowpack height, $\bar{z}_+$. 

The precision of measurements of snow depth in the data is 1 inch, and it is 0.1 inches for
SWE, creating a discretization of the target feature to 1 inch/day. High or integer discretization of
the target space hampers the ability of a regression network to learn the underlying relationships
between predictors and target. Therefore, we averaged the resulting data over a moving consecutive
$N$-day window, preserving start-of-window $z$ and SWE, accumulating precipitation, and averaging
the remaining features and target to create a denser spread in the feature space, as well as converting
units to metric where applicable. This averaging also served to smooth remaining noise and sensor
defects in the data. However, such averaging also tends to lessen extremes, which are important in
timeseries prediction (see section 2e). Because of this, we left $N$ as a hyperparameter to explore
the outcomes of these competing effects. We kept an unaveraged copy of the data, including data
with $\Delta t > 1$ day, for model performance evaluation.

To soft-constrain the network toward more physical behavior and remove data where averaging
created unrealistic values, intentional “physical” filtering was carried out on the resulting data
after averaging over $N$ days, including removing data where $z$ was nonzero but SWE = 0 (an
unphysical input), where $dz/dt > 0$ but precipitation was zero (snowpack cannot spontaneously
increase without precipitation save for local increases by wind drift, but the range of wind speeds
in the training data was predominantly under threshold speeds for snow transport found by Li and Pomeroy (1997); implying negligible influence), where \( \frac{d\text{SWE}}{dt} \) was greater than precipitation (an unphysical result as snow density must be less than or equal to water density, and the only influx of water into the system is precipitation since sites were not subject to river runoff), and where \( z < \text{SWE} \) (snowpack cannot consist of supercondensed water). Data was then excised where SWE, \( z \), and accumulated daily precipitation were all less than some small threshold \( \epsilon = 0.5 \) cm, as we wished to focus on learning snow pack evolution when snow was present, and excess zeros in the target space could drive the network to predict \( \frac{dz}{dt} = 0 \) more frequently to lower average error, precluding learning of more interesting behavior. Similarly, we removed data simultaneously satisfying \( T_{\text{air}} > 9^\circ\text{C} \) and accumulated \( \frac{dz}{dt} \) was less than \( 2\epsilon \), removing portions of the time series corresponding to summer. This heuristic for removing summer zeros was preferable to temporal filters for summer months, as the onset and disappearance of snowpacks was different for every training site and every year.

The final step was to estimate the rate \( P_{\text{snow}} \) from SNOTEL total precipitation amount (water equivalent of water and snow combined) using \( T_{\text{air}} \) and \( \varphi \), an empirical model shown to faithfully derive the water-snow phase split with over 88% accuracy (Jennings et al. 2018). The model follows

\[
f_{\text{snow}} = \frac{1}{1 + e^{\alpha + \beta T_{\text{air}} + \gamma \varphi}},
\]

with \( \alpha = -10.04 \), \( \beta = 1.41 \) \(^{\circ}\text{C}^{-1} \), and \( \gamma = 9 \) (with the relative humidity \( \varphi \in [0, 1] \)). The precipitation rate \( P_{\text{snow}} \) was then set to this fraction of the total precipitation divided by \( N \) days, and converted from in \( \text{day}^{-1} \) to \( \text{m s}^{-1} \). \( P_{\text{rain}} \), the remaining fraction of precipitation, was discarded and not used as an input feature. For application of \( M \), \( P_{\text{snow}} \) could be measured at a site, provided by renalysis data, or provided by the atmospheric model in a coupled simulation.

Features were then scaled by their standard deviations to keep all features in a similar range, and the target was scaled by its absolute maximum. These scaling constants were fixed into \( M \), to prevent the need for user manipulation of data prior to use.

**e. Training and Testing**

While achieving a small absolute error is important in predictive modeling, when accumulating predicted \( \frac{dz}{dt} \) to evolve a snowpack over time, correctly predicting extreme values holds increased
importance relative to that in other regression-learning applications due to error accumulation. For example, the integrated $z(t)$ time series may not reflect a quickly growing or depleting snowpack, causing modeled snowpacks to lag behind observations early in the winter season, or persist into the summer months and subsequently skew albedo and runoff predictions. This problem has persisted in existing physical snowpack models based on Noah, Crocus, and SNOWPACK (Gao et al. 2021; Luijting et al. 2018; Lundy et al. 2001; Wever et al. 2015; Vionnet et al. 2019). Standard regression training will often under-predict extreme values without strong target correlation or high frequencies of extreme data, both of which rarely exist in the training data. To counter these effects and promote improved predictions, extremes were emphasized by creating the custom loss function

$$L = \frac{1}{N_d} \sum_{i=1}^{N_d} w_i |y_i - \hat{y}_i|^{n_1}, \quad (4)$$

where $w_i$ is a weighting factor,

$$w_i = 1 + |y_i|^{n_2}, \quad (5)$$

and $N_d$ is the number of training examples used in the batch, $\hat{y}_i$ is the model prediction, $y_i$ is the target, and $n_1,n_2$ are constant positive integers. Optimizing a loss with $(n_1 = 1,n_2 = 0)$ and $(n_1 = 2,n_2 = 0)$ is equivalent to optimizing the average $L_1$ and $L_2$ losses, respectively. Positive $n_2$ will additionally penalize the model for poor extreme prediction without changing the convexity of the loss function since the targets are constants.

Training and hyperparameter selection of the model were carried out on a leave-one-out basis, with the averaged and filtered training data for all but one of the 37 SNOTEL sites being used as training input. The unaveraged and unfiltered ($N = 1$ and including gaps with $\Delta t > 1$ day, see section 2e.3) left-out site data was then used for scoring for hyperparameter selection. For testing the model with the optimal hyperparameter configuration, forcing data was also gathered from SNOTEL sites in Alaska, as well as additional datasets from Kühtai, Austria (Krajči et al. 2017), and Col de Porte, France (Lejeune et al. 2019). These data test the model’s ability to apply in climates outside the training set of the 37 SNOTEL sites.

Model implementation was carried out in the Julia language under the Flux framework (Innes et al. 2018; Innes 2018) and the RMSProp optimizer (Hinton et al. 2014). Training the network for 100 epochs on all training data takes less than 30 seconds on a single Intel i9 CPU with no GPU
usage, and the model storage takes up less than 4 kilobytes. Direct model evaluation scales linearly with input size in both time and memory when tested between 10 and 100000 inputs, requiring on average 1 kilobyte and 0.5 microseconds per evaluation. Linear scaling in memory and time also holds for timeseries generation. This scaling from model structure choice enables lower overhead than other more complex state-storage models like recurrent networks.

1) Evaluation metrics

Model performance was assessed both in terms of its ability to recreate targets from inputs directly (pure regression to quantify ability to learn trends in training data) as well as its ability to use its own outputs recursively in the creation of a timeseries for the entire observational period, including summers (quantifying ability under intended usage). Unlike regression predictions, which use observed snow depth inputs to predict the change in $z$ across a range of conditions to compare to observed data, the timeseries prediction utilizes the network as a neural ODE, in a self-driving manner using site data as climate forcings, where the snowpack height follows with forward Euler steps as

$$\hat{z}_{i+1} = \hat{z}_i + \Delta t M(\hat{z}_i, \text{SWE}_i, \varphi_i, R_i, v_i, T_i, P_i).$$

The resulting timeseries is evaluated against the observed timeseries. There are recent continuous adaptations of this form of discrete neural ODE (Chen et al. 2018), though such adaptations are unnecessary for this case study because the forcing data are available discretely. Evaluation metrics included mean absolute error (MAE) and root mean square error (RMSE) losses in addition to bias and residual variance, the direct regression slope between observed and predicted outputs (e.g., $m$ for $\hat{y} = my$), and the median percent error of the generated values (for timeseries, this represents the median percent error of all generated $z$ values, for pure regression, this is the median percent error of all generated $dz/dt$ values). For generated timeseries, the Nash-Sutcliffe efficiency (NSE, from Nash and Sutcliffe (1970)) was also calculated as well as an average snowpack percent error $\text{MAE}/\bar{z}_+$, where $\bar{z}_+$ is the average nonzero snowpack height. Faithful reproduction of the observed time series on out-of-sample data thus indicates valid learning of physical processes in the differential equation as well as an ability to generalize to additional climates.

We also compared the model performance against a standard linear regression model of snowpack evolution estimated from the same training data (including $z$ as a predictor, but without the inclusion
of SWE as a predictor, due to its high correlation with $z$ (Hawkins 1973)). Unlike the neural model where physical thresholds are enforced by the model and beneficially impact the training of the model weights, the linear model is estimated via least-squares, so thresholds for the linear model to enforce snowpack positivity are only enforced during the timeseries generation process in the same manner as they would be in the control flow of a larger hydrology model.

2) Snow density

Given $z$ and SWE, the snow density is known, via Eq. 1. This permits computation of a predicted snow density from the input SWE and generated $z$ timeseries, and we compared this with the similarly computed observed values. Timeseries values were only compared when observed $z$ values were nonzero. The observed data was discrete while the model output was continuous, so predicting a near-zero $z$ during nonzero observed $z$ and SWE would result in severely unphysical densities which would skew the comparison metrics and obscure interpretation of the model performance during normal snowpack conditions on average. To counter this fact, any predicted nonzero $z$ lower than the minimum observed nonzero $z$ value was treated as zero, and the resulting predicted density set to that of water. Counts and therefore frequencies of days where observed $z$ was zero and predicted $z$ was nonzero (false nonzeros), as well as days where observed $z$ was zero and predicted $z$ was nonzero (false zeros) and remaining days with unphysical densities were also recorded. This allows investigation of errors in density only during the valid snow season when density would be utilized in larger hydrology processes. The inverse relationship between $z$ and density will underscore failures of the model in the beginning and end of the snow season as well as the failure counts, since predicting minimum $z$ during an established snowpack will result in larger calculated density values, and therefore density errors. Such inflation due to the inverse relationship will also serve to skew the NSE metric as large departures from observed values accumulate in quadrature.

3) Handling gaps in data

Particular days in the unaveraged and unfiltered ($N = 1$) validation data were missing one or more input features, creating holes of varying size ($\Delta t > 1$ day) in the timeseries that prevented continuous generation by the neural model via Eq. 6. To handle these gaps and permit generation of longer continuous timeseries for benchmarking against data, holes of size $K\Delta t$ for any integer
\( K \leq K_{\text{max}} \) were traversed via

\[
\hat{z}_{i+K} = \hat{z}_i + (K \Delta t) M(\hat{z}_i, \text{SWE}_i, \varphi_i, R_i, v_i, T_i, P_i), \tag{7}
\]

and, for \( K > K_{\text{max}} \), the timeseries was “reset” via \( \hat{z}_{i+K} = z_{i+K} \), with ensuing calculations again handled by Eq. 6. Traversals resulting in negative snowpack due to the multiplication of the threshold-limited \( M \) by \( K \) were instead set to zero and allowed to continue. In this manner, the model can also be tested against its ability to surpass holes in the data in use-cases where data streams are not complete, and reduce the number of “resets” during comparison that would otherwise serve to advantageously skew performance metrics. However, keeping a maximum traversal \( K_{\text{max}} \) and maintaining snowpack positivity also prevents the accumulation of errors that are not due to the model and thereby permit a fair evaluation of performance. The number of resets on a given timeseries generation was tracked. Only 1186 gaps existed in the 103854 days of sensor data, with \( \approx 10\% \) greater than 7 days and less than 5\% greater than 30 days. Choosing \( K_{\text{max}} = 30 \) resulted in 14 sites having 0 resets, an absolute maximum of 8 resets on a timeseries of length 5116 days, and a maximum percentage of resets for 1 reset on a timeseries of length 173 days. This choice was kept for the remainder of the investigation, as preliminary testing showed smaller choices of \( K_{\text{max}} \) to lead to variations of pack percentage scores by less than 1\% on average and RMSE by less than 1 cm on average.

3. Results

a. Hyperparameter Selection

The number of averaged days \( N \), the network structural constant \( n \), and the loss function parameters \( n_1 \) and \( n_2 \) were evaluated as hyperparameters. All networks were trained over 200 epochs and a batch size of 64. Testing over \( N \in \{1, 2, 3, 4\}, n \in \{1, 2, 3, 4, 5, 6, 7, 8\}, n_1 \in \{1, 2\}, \) and \( n_2 \in \{0, 1, 2, 4\} \) with 37-fold leave-one-out cross-validation resulted in 9472 total networks trained. The loss function of each network configuration on the validation set was tracked every 10 epochs, and the best performing weight set as well as the indicative epoch was kept for evaluation and comparison to inform hyperparameter selection. As the loss function varied between hyperparameter configurations, the NSE for generated timeseries and RMSE on the validation set, both in terms
of regression on $dz/dt$ and on the generated timeseries, were the primary metrics used in judging model fitness.

We found that performance on the validation set regarding regression on $dz/dt$ was similar in magnitude to that of the training set, indicating good model generalizability. Regression performance on the validation set of $dz/dt$ values decreased with increasing $N$ (smoothing out training data and lessening extremes compared to validation values) and increased with increasing $n$ (making the model more complex) until plateauing or overfitting decreased performance around $n = 6$. Performance did not follow any discernible trends in $n_1$ but decreased for intermediary $n_2$ values with regards to direct evaluation.

However, good performance on the regression task is not sufficient to guarantee performance in the generation of timeseries, as small errors from poor predictions of extremes or overfitting can accumulate over time. Table 1 and Fig. 4 show the averaged model scores over particular $(n_1, n_2)$ and $(N, n)$ configurations. The variation between most configurations is on the order of a few percent, and the variations are suppressed by averaging over all subconfigurations; however, the timeseries error is smallest at a value of $n_2 = 1$, weakly validating the emphasis of extreme points in the loss function. Increasing $n$ (which controls the size of the network) beyond intermediary values for any $N$ does not yield any change in performance.

Table 1. Performance metrics of the generated timeseries for a particular $(n_1, n_2)$ configuration. Notice that $(1, 0)$ is the standard average $L_1$ norm and $(2, 0)$ is the standard average $L_2$ norm. These are averaged over the choices of $N, n$ and over the 37-fold cross-validation, which serve to lessen the variation across the variables. The median percent error is exaggerated relative to pack percent error due to overprediction when $z$ is small.

<table>
<thead>
<tr>
<th>$(n_1, n_2)$</th>
<th>MAE ($m$)</th>
<th>RMSE ($m$)</th>
<th>NSE</th>
<th>Median Series Err. (%)</th>
<th>Median Regression Err. (%)</th>
<th>Pack Err. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1, 0)</td>
<td>0.0619</td>
<td>0.105</td>
<td>0.926</td>
<td>16.7</td>
<td>59.0</td>
<td>8.45</td>
</tr>
<tr>
<td>(1, 1)</td>
<td>0.0608</td>
<td>0.103</td>
<td>0.930</td>
<td>16.3</td>
<td>58.3</td>
<td>8.30</td>
</tr>
<tr>
<td>(1, 2)</td>
<td>0.0614</td>
<td>0.104</td>
<td>0.929</td>
<td>16.6</td>
<td>58.9</td>
<td>8.39</td>
</tr>
<tr>
<td>(1, 4)</td>
<td>0.0619</td>
<td>0.105</td>
<td>0.927</td>
<td>16.7</td>
<td>59.1</td>
<td>8.43</td>
</tr>
<tr>
<td>(2, 0)</td>
<td>0.0643</td>
<td>0.108</td>
<td>0.924</td>
<td>17.2</td>
<td>57.1</td>
<td>8.78</td>
</tr>
<tr>
<td>(2, 1)</td>
<td>0.0624</td>
<td>0.105</td>
<td>0.929</td>
<td>16.7</td>
<td>56.8</td>
<td>8.52</td>
</tr>
<tr>
<td>(2, 2)</td>
<td>0.0634</td>
<td>0.107</td>
<td>0.927</td>
<td>17.0</td>
<td>57.3</td>
<td>8.64</td>
</tr>
<tr>
<td>(2, 4)</td>
<td>0.0639</td>
<td>0.107</td>
<td>0.924</td>
<td>17.2</td>
<td>57.3</td>
<td>8.72</td>
</tr>
</tbody>
</table>
Fig. 4. Nash-Sutcliffe Efficiency of the generated timeseries for a particular $N, n$ configuration. These are averaged over the choices of $(n_1, n_2)$ and over the 37-fold cross-validation, which reduces the variation across the variables. Unlike the training and validation errors, the patterns are more complex and find that particular configurations perform better than others for timeseries generation.

The hyperparameter configuration with the lowest timeseries error had $N = 1$, $n = 5$, $n_1 = 1$, $n_2 = 1$ when trained for 100 epochs. We maintained this configuration for further investigation of performance. This model configuration was able to generate snowpack timeseries with under 7% error in most cases with an absolute bias of under a centimeter and with Nash-Sutcliffe Efficiencies of over 0.97. Full performance statistics of the model configuration are given in Table 2.

b. Optimal Model Performance on Test Data

The performance of the model across 5 Alaskan testing sites, as well as the France and Austria sites, are summarized in Table 3. The model performs much more consistently across the testing sites than the cross-validation sites. The model shows $\approx 9\%$ average error on total snowpack prediction with a RMSE of 10 centimeters and a MAE of about 6 centimeters, which is on par with or smaller than established models and other more complex models during testing (Vionnet et al. 2012; Brun et al. 2013; Viallon-Galinier et al. 2020; Luijting et al. 2018; Ebner et al. 2021; Meloche et al. 2022; Gao et al. 2021; De Michele et al. 2013a). These established models do not take observational SWE as input, but are either full hydrology models (compared to $M$’s intended
Table 2. Statistics of the best-performing model ($N = 1, \ n = 5, \ n_1 = 1, \ n_2 = 1$) with regards to timeseries prediction across all 37-fold cross-validations. All performance statistics also show that the median is better than or equal to the mean, suggesting more isolated cases of less performance and better generalizability.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE ($m$)</td>
<td>0.0110</td>
<td>0.251</td>
<td>0.0532</td>
<td>0.0480</td>
</tr>
<tr>
<td>RMSE ($m$)</td>
<td>0.0282</td>
<td>0.394</td>
<td>0.0907</td>
<td>0.0775</td>
</tr>
<tr>
<td>NSE</td>
<td>0.652</td>
<td>0.989</td>
<td>0.949</td>
<td>0.970</td>
</tr>
<tr>
<td>Bias ($m$)</td>
<td>-0.251</td>
<td>0.121</td>
<td>-0.0126</td>
<td>0.0086</td>
</tr>
<tr>
<td>$\sigma_{resid}(m)$</td>
<td>0.0282</td>
<td>0.304</td>
<td>0.0846</td>
<td>0.0730</td>
</tr>
<tr>
<td>Regression Slope</td>
<td>0.549</td>
<td>1.100</td>
<td>0.954</td>
<td>0.962</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>4.10</td>
<td>69.0</td>
<td>14.7</td>
<td>11.9</td>
</tr>
<tr>
<td>Median Regression Err (%)</td>
<td>40.1</td>
<td>100.0</td>
<td>58.1</td>
<td>55.8</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>4.30</td>
<td>24.8</td>
<td>7.21</td>
<td>6.25</td>
</tr>
</tbody>
</table>

role as a subcomponent within such a model, and would utilize their predicted $SWE$ values), or input historical snow depth data such as the mean annual snow depth. Yet, our ML model does not require history of a snow states or storage of microphysical states to achieve similar results. The model also shows about $3\times$ lower error than the linear model across the same tests (summarized in Table 4), indicating the linear parameterization does not generalize as well even when trained on the same data. The plots in Fig. 5 show the neural model also performs better at growing and depleting the snowpack at pace with observations, while the linear parameterization tends to lag into the summer months or lag on sufficient growth speed, or create snowpacks inbetween seasons.

Figure 6 displays the resulting timeseries from using generated snowpack evolution to calculate bulk density, and Table 5 shows the numerical comparison of estimated bulk density against observations over all 7 testing sites. The neural model still outperforms the linear model in this regard and now by a factor of about 5 (compare the linear model results in Table 6). Without an explicit constraint preventing $z$ from decreasing below a newly-updated SWE, the neural model occasionally predicts a new $z$ that is less than the new SWE during small snowpacks, which causes a large density error, though on average the model can predict observed density to under 25% error.
Fig. 5. Subsets of the generated timeseries by the neural model and the linear model. The neural model outperforms the linear parameterization when tested out-of-sample, while the linear model tends to create snowpacks during summer months or lag on growth or decay relative to observations.

c. **Model Dissection**

1) **Model Residuals**

In order to assess bias in the model, we looked at correlations between predicted and true values of $dz/dt$ and between the residuals and the predicted values. Fig 7 shows the results for the neural and linear models. The correlation score for predicted vs true values for the neural model is $r = 0.77$, while the linear model shows a correlation score of $r = 0.70$. Both models continue to show a tendency to under-predict extreme values and perform similarly on rarer extreme events, though the neural model performs with smaller residuals for small-magnitude events, especially for decreases in $z$.

Both models show no discernible trends in the residuals vs. the output value, but they tend to still under-predict the magnitude of extreme values. This may be because the models were exposed to
Table 3. Performance of the neural model across all 7 testing sites. Including the sites with highly varied scoring from validation has lowered the variance of performance of the model over the test cases and improved the ability of the model to generalize to different climates. The median is now much closer to the mean, implying a more normal spread in behavior for a given climate.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (m)</td>
<td>0.0256</td>
<td>0.098</td>
<td>0.0620</td>
<td>0.0712</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.0450</td>
<td>0.1615</td>
<td>0.107</td>
<td>0.1197</td>
</tr>
<tr>
<td>NSE</td>
<td>0.850</td>
<td>0.983</td>
<td>0.940</td>
<td>0.945</td>
</tr>
<tr>
<td>Bias (m)</td>
<td>-0.070</td>
<td>0.091</td>
<td>-0.0151</td>
<td>-0.0175</td>
</tr>
<tr>
<td>$\sigma_{\text{resid}} (m)$</td>
<td>0.0414</td>
<td>0.1336</td>
<td>0.0966</td>
<td>0.1018</td>
</tr>
<tr>
<td>Regression Slope</td>
<td>0.849</td>
<td>1.200</td>
<td>0.941</td>
<td>0.916</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>8.47</td>
<td>28.70</td>
<td>14.98</td>
<td>14.93</td>
</tr>
<tr>
<td>Median Regression Err (%)</td>
<td>50.4</td>
<td>71.0</td>
<td>60.9</td>
<td>66.1</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>5.17</td>
<td>16.23</td>
<td>9.03</td>
<td>8.57</td>
</tr>
</tbody>
</table>

Table 4. Performance of the linear model across all 7 testing sites. The poor performances indicated by the maximums and minimums are indicative of the inability of the parameterized model to generalize, even though it is trained on the same data as the neural model.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (m)</td>
<td>0.0610</td>
<td>0.3241</td>
<td>0.2006</td>
<td>0.1987</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.1123</td>
<td>0.4805</td>
<td>0.3264</td>
<td>0.3374</td>
</tr>
<tr>
<td>NSE</td>
<td>0.3173</td>
<td>0.6940</td>
<td>0.5204</td>
<td>0.5153</td>
</tr>
<tr>
<td>Bias (m)</td>
<td>-0.3240</td>
<td>0.1381</td>
<td>-0.1071</td>
<td>-0.0932</td>
</tr>
<tr>
<td>$\sigma_{\text{resid}} (m)$</td>
<td>0.1010</td>
<td>0.3550</td>
<td>0.2747</td>
<td>0.3207</td>
</tr>
<tr>
<td>Regression Slope</td>
<td>0.4051</td>
<td>0.6395</td>
<td>0.7367</td>
<td>0.6527</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>34.49</td>
<td>63.95</td>
<td>46.01</td>
<td>44.23</td>
</tr>
<tr>
<td>Median Regression Err (%)</td>
<td>46.3</td>
<td>59.7</td>
<td>54.4</td>
<td>55.3</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>20.45</td>
<td>32.98</td>
<td>27.41</td>
<td>29.66</td>
</tr>
</tbody>
</table>

more data near small values of $dz/dt$, which could lead to better predictions of smaller values at the expense of extremes.

2) Feature Importance of Neural Model

Table 7 shows the feature importance of each predictive variable, equal to the percentage increase in RMSE when the given feature is randomly shuffled, for both direct (regression) predictions as well as when generating timeseries. The wind speed and $\varphi$ remain relatively unimportant in both
Fig. 6. Density plots for two of the same timeseries from Fig 5. The neural model again outperforms the linear model, though both occasionally lag in snowpack prediction at the start or end of the season, creating spikes at the beginning and end of each season which will serve to skew the Nash-Sutcliffe statistic. Discontinuity comes from the corner cases described in section 2e.2.

Table 5. Performance statistics for the model’s generation of density timeseries. The large point-errors for predicting $z < \text{SWE}$ as well as incorrectly predicting the snow season start or end skew the Nash-Sutcliffe score, but the model shows an ability to recreate density with an error of about 25%.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE ($\text{kg m}^{-3}$)</td>
<td>0.0396</td>
<td>0.1174</td>
<td>0.0723</td>
<td>0.0671</td>
</tr>
<tr>
<td>RMSE ($\text{kg m}^{-3}$)</td>
<td>0.0846</td>
<td>0.2616</td>
<td>0.1577</td>
<td>0.1660</td>
</tr>
<tr>
<td>Bias ($\text{kg m}^{-3}$)</td>
<td>-0.1046</td>
<td>0.0665</td>
<td>0.0075</td>
<td>0.0016</td>
</tr>
<tr>
<td>$\sigma_{\text{resid}}$ ($\text{kg m}^{-3}$)</td>
<td>0.0829</td>
<td>0.253</td>
<td>0.1499</td>
<td>0.1336</td>
</tr>
<tr>
<td>Regression Slope</td>
<td>0.687</td>
<td>1.259</td>
<td>1.012</td>
<td>1.029</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>8.94</td>
<td>21.8</td>
<td>14.86</td>
<td>16.77</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>15.56</td>
<td>32.16</td>
<td>24.49</td>
<td>26.23</td>
</tr>
<tr>
<td>False Zeros (%)</td>
<td>0.30</td>
<td>0.86</td>
<td>0.61</td>
<td>0.83</td>
</tr>
<tr>
<td>False Nonzeros (%)</td>
<td>0.67</td>
<td>4.64</td>
<td>2.01</td>
<td>1.97</td>
</tr>
<tr>
<td>Unphysical Density (%)</td>
<td>0.0</td>
<td>0.96</td>
<td>0.29</td>
<td>0.03</td>
</tr>
</tbody>
</table>

cases, and for reduced complexity both can be removed from the model or imputed without loss of accuracy (see section 3d). SWE becomes more important for generation of timeseries and becomes the predominant predictor variable, while $z$ itself becomes less important. The reduction in the importance of $z$ in timeseries generation suggests a robustness of the model to accumulated errors since better $dz/dt$ values are predicted even under an input of incorrect $z$ in the timeseries case vs. the regression case, which likely help it succeed over the linear regression model. It is also
Table 6. The performance of the linear parameterization on the testing sites for bulk density timeseries. Errors are roughly five times that seen in the neural model, and the linear model is considerably worse with regard to false zeros, false nonzeros, and predicting unphysical densities.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (kg m(^{-3}))</td>
<td>0.0200</td>
<td>0.8074</td>
<td>0.0395</td>
<td>0.0286</td>
</tr>
<tr>
<td>RMSE (kg m(^{-3}))</td>
<td>0.0466</td>
<td>1.927</td>
<td>0.987</td>
<td>0.661</td>
</tr>
<tr>
<td>Bias (kg m(^{-3}))</td>
<td>-0.050</td>
<td>0.727</td>
<td>0.275</td>
<td>0.220</td>
</tr>
<tr>
<td>(\sigma_{residuals}) (kg m(^{-3}))</td>
<td>0.428</td>
<td>1.785</td>
<td>0.937</td>
<td>0.649</td>
</tr>
<tr>
<td>Regression Slope</td>
<td>0.826</td>
<td>3.649</td>
<td>2.027</td>
<td>1.949</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>32.74</td>
<td>123.27</td>
<td>64.20</td>
<td>53.40</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>48.90</td>
<td>292.60</td>
<td>142.08</td>
<td>126.99</td>
</tr>
<tr>
<td>False Zeros (%)</td>
<td>0.95</td>
<td>8.70</td>
<td>5.26</td>
<td>5.83</td>
</tr>
<tr>
<td>False Nonzeros (%)</td>
<td>0.0</td>
<td>10.58</td>
<td>2.93</td>
<td>1.75</td>
</tr>
<tr>
<td>Unphysical Density (%)</td>
<td>1.04</td>
<td>12.57</td>
<td>5.41</td>
<td>4.05</td>
</tr>
</tbody>
</table>

Table 7. Relative error scores generated in both direct prediction and timeseries generation for a random shuffling of the feature. The reported scores show the averages calculated over 10 random shufflings per feature while keeping other features constant. The higher the number, the larger an impact that feature has on the model output in a direct regression or accumulated time-stepping setting.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Direct Score</th>
<th>Series Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>(z)</td>
<td>3.832</td>
<td>1.227</td>
</tr>
<tr>
<td>SWE</td>
<td>3.406</td>
<td>5.413</td>
</tr>
<tr>
<td>(\phi)</td>
<td>1.082</td>
<td>1.101</td>
</tr>
<tr>
<td>(R)</td>
<td>1.301</td>
<td>2.027</td>
</tr>
<tr>
<td>(v)</td>
<td>1.012</td>
<td>1.002</td>
</tr>
<tr>
<td>(T)</td>
<td>1.352</td>
<td>3.804</td>
</tr>
<tr>
<td>(P)</td>
<td>1.559</td>
<td>2.070</td>
</tr>
</tbody>
</table>

observed that insolation, temperature, and precipitation hold increased importance in timeseries generation relative to their direct regression counterparts.

3) Physical Behavior of Model

In order to interpret how the model makes a prediction, we considered the model output as a function of air temperature and either precipitation or insolation, for fixed values of the other variables and at fixed snow depth.
Fig. 7. Predicted vs. observed targets and residuals against the modeled target by the neural and linear models. Both models continue to under-predict extremes, but the neural model performs slightly better in this regard than the linear model.

In Fig. 8a, we see that, when air temperatures are below freezing, increasing the snowfall produces an increase in $dz/dt$, in an approximately linear fashion (i.e., contours becoming more evenly spaced and less curved). Above the freezing temperature, the snowfall rate needs to be larger to produce the same $dz/dt$. At some point, for low enough precipitation rates and warm enough temperatures, $dz/dt$ is negative, in accordance with physical expectations. Interesting behaviors occur in some regimes, as the no-growth ($dz/dt = 0$) contour dips with increasing precipitation in the $T - P_{\text{snow}}$ plane as opposed to the expected flat behavior otherwise for an average winter day ($R \approx 60$ W m$^{-2}$ averaged across site data in February) with small snowpacks. Likewise, the inability of all contours to become fully vertical at colder temperatures implies there is no learned minimum density of accumulated snowfall, though most contours become do increasingly vertical for colder temperatures. Since these behaviors persists for larger snowpacks (the plot was generated
for a shallow snowpack), this can be reinterpreted as regions of space where the model failed to
fully learn the expected representation and would benefit from additional training data in these
regimes to better encapsulate the required effects.

Figure 8b considers the case of how air temperature and insolation affect snow depth, at zero
snowfall. We see that snowpack depletion begins shortly after average air temperature increases
above freezing, as well as for increasing insolation. It also reflects an inability of the snowpack to
grow under a lack of snowfall, as all output values are nonpositive.

The variable spacing of contours also indicates a learning of nonlinear behavior, as opposed to a
linear regression model, which will have linear and evenly spaced contours everywhere in parameter
space. The contours are also not entirely smooth due to the choice of activation functions, which
have discontinuous derivatives.

The model thresholds also prevent the snowpack from decreasing to a negative value, showcas-
ing an ability to replicate physical behaviors as well as physical limitations. Likewise, growth
contours shift in the negative direction with increasing wind-speed (indicating a learning of wind-
compaction; not shown), and slightly shift in the positive direction for increasing relative humidity
(not shown).

**Fig. 8.** Example outputs from the model over two sets of snowpack conditions. In each case one threshold
condition is visible, i.e., where the snowpack cannot deplete beyond its starting value, and cannot grow without
snowfall.
4) Generalizability

Figure 9 shows the elevation vs. mean nonzero snowpack height $\bar{z}_+$ scatterplots for all training and all seven testing sites in a similar manner to Fig. 3, though the sites are now colored by the performance of $M$ for pack percentage error on $z$ and pack percentage error on density (equal to the MAE of the density timeseries divided by the average true density value), as well as direct RSME and NSE on computed timeseries.

The model performs well comprehensively with regards to pack percentage error on $z$, with less than a 20% error on all sites and most sites under 10%, while density errors are higher by roughly a factor of 4–5 (though these averages are inflated by individual extreme densities at the beginning and end of the prediction season, as is visible in Fig. 6). The model also performs similarly on the available testing site data compared to the training data, which covers much lower
elevations than the training data, as well as the smallest average nonzero snowpack height, implying a strong ability to generalize to out-of-sample regimes, even for density calculations. No trend with elevation appears in the results, corroborating generalizability rather than elevation-induced indirect effects.

5) Threshold Importance

Our model employs two thresholds for snowpack evolution, which prevent accumulation under no precipitation and prevent the loss of more snow than exists in the snowpack. Figure 10 shows the result of the neural and linear models when no thresholds are implemented within the training nor in the control flow of timeseries generation on a testing site in Alaska, with no gaps in the forcing data. Without the threshold designed specifically to prevent snowpack height from becoming negative, both models predict negative heights in the summer, though this error is worse for the linear model. This happens in every generated timeseries for all models. Without the threshold designed to prevent accumulation of snow without precipitation, the neural model predicts an increase in the snowpack height for 2.7% of forcing inputs where no snow precipitation occurs. Both types of errors are unphysical. Without thresholds, the average RMSE of the neural model on generated

Fig. 10. Performance of both models when thresholding is not enforced. Behavior is similar across all testing and training sites, this site requires no timeseries resets, so all negative snowpacks are entirely created by the model.
timeseries increases by two centimeters and the pack percentage error increases by 3%, implying that the thresholds weakly improve performance in addition to maintaining adherence to physical constraints.

\[ \text{d. Model adaptability and variability} \]

1) **Reduced Variable Set**

The results of section 3c.2 suggest that wind speed is not an important variable for enabling model performance, so additional SNOTEL sites without wind speed data can also be tested for additional validation by imputing the wind speed input with the constant average of the training data. Furthermore, the remaining input features without wind speed data can be entirely inferred from satellite feeds, increasing the usability of the learned model in real-world settings or simpler hydrology models without requiring the assimilation of multiple data sources. As relative humidity was the second least important variable, the performance under the removal of this variable as well can be tested for an overall further reduction in model complexity.

Table 8 shows the results over four additional testing sites in Alaska with the mean wind speed imputed, with the mean wind speed and the mean relative humidity imputed, as well as the results when training an entirely new network without the wind speed or relative humidity variables. The Table 8. Scores of model \( M \) when run on additional testing sites without wind speed or relative humidity as predictors. Performance of the model is roughly the same in all cases and suggests that removing predictors instead of imputing them is a beneficial choice due to similar performance but with further reduced computational complexity.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Impute ( v )</th>
<th>Impute ( v, \phi )</th>
<th>No ( v, \phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (m)</td>
<td>0.0598</td>
<td>0.0644</td>
<td>0.0556</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.1097</td>
<td>0.1120</td>
<td>0.0979</td>
</tr>
<tr>
<td>NSE</td>
<td>0.938</td>
<td>0.943</td>
<td>0.960</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>12.08</td>
<td>13.17</td>
<td>13.09</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>8.06</td>
<td>8.50</td>
<td>7.36</td>
</tr>
</tbody>
</table>

Performance scores of \( M \) under all scenarios are nearly identical to those presented in Table 3 and to each other. That is, removing these features vs. imputing them does not significantly impact performance relative to their inclusion, even on out-of-sample data in new climates.
The ability to perform under missing variables extends the usability of the model under situations where data are not available or gaps exist at a given site or simulation, as well as further reduces the model complexity. The ability to add, remove, and impute features under the modular assembly of the model is straightforward.

2) Finer Resolution Predictions

The only terms in $M$ containing units of time are the input precipitation, the output, and the lower threshold on the output, all of which are rates. The prediction of rates $dz/dt$ instead of solely accumulated $dz$ over a predetermined time step means the model can be tested at time steps that differ from the time increment of the data it was trained with, without retraining of the model. The site data from Kühtai contains resolution at 15-minute intervals, allowing the model to be evaluated at weekly, daily, hourly, and 15-minute resolution, of which the results are displayed in Fig. 11 and Table 9.

Table 9. Performance of the model $M$ at different time resolutions. There is a jump in error when departing from the resolution the model was trained at, but performance remains near-constant between hourly and 15-minute resolution.

<table>
<thead>
<tr>
<th>Statistic/Resolution</th>
<th>Weekly</th>
<th>Daily</th>
<th>Hourly</th>
<th>15-Minute</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (m)</td>
<td>0.0895</td>
<td>0.0645</td>
<td>0.1143</td>
<td>0.1181</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.1527</td>
<td>0.1134</td>
<td>0.1882</td>
<td>0.1950</td>
</tr>
<tr>
<td>NSE</td>
<td>0.901</td>
<td>0.945</td>
<td>0.849</td>
<td>0.838</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>21.06</td>
<td>14.92</td>
<td>27.01</td>
<td>27.54</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>11.90</td>
<td>8.57</td>
<td>15.24</td>
<td>15.73</td>
</tr>
</tbody>
</table>

The timeseries generated with the four different timesteps are shown in Fig 11. There is an increase in the error when the timestep is both larger or smaller than $\Delta t = 1$ day, the value the model was trained with. However, the error does not significantly worsen when moving from an hourly to a 15-minute temporal resolution. This loss of performance may be due to the range of values for $dz/dt$ and precipitation seen at higher-resolution and more coarsely grained data. While the daily data might show snowpacks increasing a few centimeters over a day, the finer resolution may show the same total deposition over a few-hour period (more extreme values of $P$), resulting in values of $dz/dt$ that are 10–20× larger in magnitude than those present in the daily training data. Likewise, at the weekly scale, true observed extreme events that drive extremes in outputs are
driven to smaller forcing inputs by averaging, while the accumulation of fine-resolution extreme events in the observed data is manifested in the start-of-week (not weekly averaged) observed $z$ values. The linear model, on the other hand, is more robust to resolution changes and has roughly constant performance across resolution changes; however, it is worse in all regards compared with the full model $M$. The performance of the neural model demonstrates an ability to generalize to other temporal resolutions, but performance would likely be improved if the training data contained a larger range of $dz/dt$ training values (for instance, by including both hourly and daily resolution training data).

3) **Alternative Use-Cases**

The SNOTEL data contains both SWE and snow depth; we chose to use SWE as input to a model for $dz/dt$ in anticipation of use within a bulk snow model, where SWE is modeled prognostically using conservation laws. An alternative use-case is predicting available snow water content (SWE) in summer months following snowmelt of snowpacks with measured depths.

By swapping SWE and $z$ features, the model can be retrained to instead predict $dSWE/dt$ when provided $z$ data. We carried out this experiment with no further changes to the training pipeline. The results on all seven testing sites for training the retrained model (delineated as $M'$) on the 37 SNOTEL sites to instead predict $dSWE/dt$ are shown in Table 10. The results are also repeated for using $M'$ and removing both relative humidity and wind speed variables in the same manner as...
in section 3d.1, resulting in a reduced model (now labeled $M''$) $d\text{SWE}/dt = M''(\text{SWE}, z, R, T, P)$ which is also shown in Table 10.

**Table 10.** Results over all seven testing sites by instead training the chosen model structure to predict $d\text{SWE}/dt$ given $z$ instead of $dz/dt$ given SWE, under a full and reduced set of variables. Hyperparameter testing was not carried out for this case; further improvement could be gained by doing so.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>$M'$</th>
<th>$M''$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE (m)</td>
<td>0.0231</td>
<td>0.0222</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.0380</td>
<td>0.0380</td>
</tr>
<tr>
<td>NSE</td>
<td>0.922</td>
<td>0.921</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>19.70</td>
<td>20.04</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>11.44</td>
<td>11.11</td>
</tr>
</tbody>
</table>

The model can predict SWE timeseries with an average RMSE of under 4 cm and with average NSE scores of over 0.92, with an average percentage error of about 11%, which is still improved relative to previously cited models. The performance of this model given performance for predicting $dz/dt$ is not surprising given the high correlation between $z$ and SWE or between $dz/dt$ and $d\text{SWE}/dt$, though the model performs better for $z$ prediction than SWE prediction with regard to pack percentage error. However, the SWE prediction model generalizes about as well as the $z$ model, with pack percentage errors ranging between 7% and 17% for SWE as opposed to 5% and 16% for $z$, but this could again likely be improved with hyperparameter exploration, and at a minimum offers a starting point for future studies.

A final case study to test the limits of the model is evaluating its capability for a standalone fully data-driven bulk snowpack model, where two networks $M_z$ and $M_{\text{SWE}}$ separately trained drive snowpack prediction in a coupled manner, according to

$$\bar{\text{SWE}}_{i+1} = \text{SWE}_i + \Delta t M_{\text{SWE}}(\hat{z}_i, \bar{\text{SWE}}_i, \varphi_i, R_i, v_i, T_i, P_i),$$

(8)

and

$$\hat{z}_{i+1} = \hat{z}_i + \Delta t M_z(\hat{z}_i, \bar{\text{SWE}}_i, \varphi_i, R_i, v_i, T_i, P_i),$$

(9)

with adaptations as described in Eq. 7 for gaps in the data. Alternative choices could include training weights simultaneously under a combined loss function or pairing both outputs into one
model, but both introduce additional tradeoffs between \( z \) and SWE predictions for only a minimal reduction in complexity. This setup would provide a fast and low-resource model for generating \( z \), SWE, and bulk density and therefore all subsequently derived quantities, requiring only atmospheric variables and initial values \( z_0 \) and SWE\( _0 \) (which can be simply initialized at zero and started during the summer for many locations). The only change in this case to ensure respect of physical laws is to alter the lower threshold of \( M_z \) such that the update of \( z \) follows \( z_{i+1} \geq \text{SWE}_{i+1} \) to enforce \( z \geq \text{SWE} \).

Table 11. Performance of the coupled model run as a standalone bulk hydrology model over the seven testing sites, with full and reduced set of input features.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>With ( v, \phi )</th>
<th>No ( v, \phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( z )</td>
<td>SWE</td>
</tr>
<tr>
<td>MAE (m)</td>
<td>0.1149</td>
<td>0.0369</td>
</tr>
<tr>
<td>RMSE (m)</td>
<td>0.1908</td>
<td>0.0635</td>
</tr>
<tr>
<td>NSE</td>
<td>0.835</td>
<td>0.843</td>
</tr>
<tr>
<td>Median Series Err. (%)</td>
<td>24.11</td>
<td>23.97</td>
</tr>
<tr>
<td>Pack Err. (%)</td>
<td>15.54</td>
<td>15.97</td>
</tr>
</tbody>
</table>

Fig. 12. Two example timeseries from the coupled prediction models with the full set of input variables, with one better example in Alaska and a poorer example from France. The offset in \( z \) is correlated with the offset in SWE.

The results of this system both under the full set of predictor variables as well as under the reduced set (without relative humidity nor wind speed) on the seven testing sites are shown in Table 11 and displayed (for the full variable set) in Fig. 12. As errors are accumulating from both
and SWE under this scheme, it is unsurprising to see increased average errors in both variables and their timeseries relative to their standalone cases, but by less than a factor of 2. Similarly, the generalizability of the combined model is further reduced under accumulated errors, with pack percentage errors from the full set of input variables ranging from 9% to 30% for $z$ and 9% to 23% for SWE. However, on average model pack percentage errors are still close to previously cited models with 15% average snowpack error, for a fraction of the computational cost. The medians of every statistic were lower than their average (save for NSE, which was higher), and did not significantly change with the inclusion of the performance metrics on the training sites, implying fair performance at low overhead for over 20 sites from many different seasonal climates. This combined model under the full set of input features also creates density timeseries with an MAE of 6.7 kg m$^{-3}$, a RMSE of 12.8 kg m$^{-3}$, and a mean timeseries percentage error of 23%, again less than double the errors in the standalone case. The errors on SWE predictions are also closer to their standalone errors than those of $z$ predictions, implying the predictive capability of $M$ is more reliant upon accurate SWE prediction than $z$, which is in line with the results of the feature importance seen in Table 7. As both models were trained with only the final hyperparameter selection for best $z$ prediction, further improved predictions in coupled form is likely with little more than hyperparameter tuning for SWE prediction or substitution with another more accurate SWE model. Such an investigation remains for future study, but the existing results serve to showcase both the utility and versatility of the presented model structure. In particular, the capability under reduced inputs opens avenues for real-world benefit under minimal data availability or with low computational resources (see section 4).

4. Discussion

The overarching aim of this study was to explore using a simple and versatile data-driven model to predict snow depth (or density) while maintaining or superseding contemporary predictive capabilities. The rationale offered in model construction and data choice and cleaning were largely results-driven and focused on seasonal snowpack forecasting across locations and climates. For instance, choosing variables that are easily and widely measured/inferred widens model applicability as well as its ability to be benchmarked for generalizability. However, requiring complete atmospheric, meterological, and ground-based input features at simultaneous locations and times
pruned sources for training data to the daily resolution of the SNOTEL network, which was not quality-controlled to the extent seen for the the Kühntai and Col De Porte datasets. Less quality control in tandem with deliberately minimal data cleaning suggests the model was trained on noisy data, which likely impacts final model weights and subsequent performance for both $M$ and its linear counterpart. Availability of widespread quality-checked data at finer resolutions like those from Kühntai would have increased the range of extremes present for training and likely further improved performance across temporal resolutions. While the inclusion of reanalysis data was considered for this purpose, this idea was discarded due to concern $M$ would merely relearn reanalysis parameterizations rather than potentially recreate measured natural effects, informing the choice of solely primary source data. The requirement of flat open territory for snow pillows and sensor networks also implies the model was never evaluated against fractal-like terrain, with crevices shaded from insolation or mountainsides perpendicular to wind. The same goes for tundra and taiga biomes with perpetual snow cover and strong winds where drift effects are significant. The model’s extrapolation to such unsampled terrains is unknown, and thus the ability of $M$ to be utilized truly “globally” remains an open question. Further appraisal of the presented model type under future data streams in a world of growing data volume, frequency, and quality offers an exciting avenue for future research.

The best configuration for timeseries generation had different hyper-parameters than that for direct regression on validation data. This underscores that the ability to better predict $dz/dt$ in general does not guarantee better recreation of accumulated seasonal timeseries. This further supports the idea that our chosen model, loss function, and time- and location-independent input features, is learning something beyond the matching of magnitudes and is summarizing the effects of inherently universal and memoryless natural/physical processes. In particular, the model only began to fail when new climates presented target magnitudes that were not well-reflected in the training data, instead of when presented snowpacks with different input feature magnitudes from those in the training data. Generalizability of output magnitude is poor, as with many data-driven models, but, the input generalizability is a beneficial and less common result highlighting the benefit of seeking physical realizability of the model. This also accentuates the benefit of attaining widespread localized seasonal snow sensing across varying (or extreme) climates to enhance the predictive power of such models.
The model’s capabilities and its modularity for handling the addition or removal of data streams showcase a wide range of possible extensions. In particular, this facilitates straightforward and synergistic integration as a “plug-and-play” prognostic model inside physics-based hydrology suites that predict SWE, due to $M$’s sensitivity to SWE and also its respect of physical constraints and linear computational overhead after one-time training. The model $M$’s ability to run year-round at any input-defined spatial and temporal resolution with low computational cost can significantly reduce bottlenecks while still offering similar or improved accuracy to more advanced models, permitting predictions longer into the future or at finer resolutions. The modularity also enables its ability to act as a standalone predictive model wherever inputs can be measured or inferred even where no historical records exist. This permits real-world utility for nowcasting applications with economic implications, such as weekly skiing or hiking terrain predictions from weather forecasts for tourism or maintenance, or annual water supply forecasting in areas reliant on snowmelt.

Beyond tuning $M$ for SWE prediction and testing $M$ in a combined setting with an improved SWE model or entire hydrology model, other future directions of inquiry could involve the adaptation of $M$ to continuous neural ODE structures and how to enforce absolute (and resolution-dependent) constraints on these structures or more general timestepping schemes. Opportunities for improving data methods include augmenting the model with additional data streams containing depth data, such as NOHRSC data or additional SNOTEL sites, to model snow layers or temperature profiles. Likewise, incorporating pressure data estimated from nearby weather stations could improve model output and would indirectly encode elevation-based effects into $M$, and likely further improve the model’s ability to generalize. Alternative training methodology could include using generated timeseries error as the loss function and gradient-free update rules to avoid gradients of the recursively generated timeseries values.

5. Conclusion

Using a location-agnostic and physically constrained neural network within an ODE as a model for the rate of change of snow depth, we were able predict seasonal snow depth with a typical error of 9% across sites with varying climates and elevations, including some not seen during training. Though the model was trained with daily data, it shows an ability to perform with comparable accuracy at other temporal resolutions without additional retraining of the model. The model’s structure
reduces computational overhead while maintaining performance compared to memory-based models or those requiring tracking of microscale processes to reproduce macroscale observations. This shows an ability to better represent universal processes than other parameterizations despite its own data-driven nature.

The design of the model enables straightforward integration into more complex snow models that require a prognostic treatment of snow depth or can be adapted to alternatively forecast variables like snow water content. As a standalone measure when fed with observational SWE and meteorological data, the model can recreate seasonal timeseries with more than a 20% improvement over other models. It is similarly able to match contemporary performance standards even when augmented to simultaneously predict its own inputs, offering multiple applications for both long-term climate simulations as well as immediate real-world applications.

The general structure of the model and the means of enforcing hard constraints via the model structure offer a simple but powerful technique for predictive modeling with utility that extends beyond snowpack modeling. In particular, it is easily adaptable to different predictive scenarios, which increases both the model’s usability and preserves its relevance for future or similar challenges.
Acknowledgments. The authors thank Marie Dumont for insightful discussions about process-based snow models and the SNOTEL effort and the teams from the Kühtai and Col De Porte stations for providing the snow sensor data. A. C. was supported by the AI4Science initiative at the California Institute for Technology and a Department of Defense National Defense Science and Engineering Graduate (NDSEG) Fellowship. This work was also generously supported by Eric and Wendy Schmidt (by recommendation of Schmidt Futures).

Data availability statement. The SNOTEL data utilized in this study was available via the National Water and Climate Center, which lies under the United States Department of Agriculture. Data reports of the SNOTEL data were generated using the online portal found at https://www.nrcs.usda.gov/wps/portal/wcc/home/. The data from Col De Port (Lejeune et al. 2019) can be found at the Observatoire des Sciences de l’Univers de Grenoble DOI portal https://doi.osug.fr/public/CYOBSCCLIM_CDP/CYOBSCCLIM.CDP.2018.html, and data from Kühtai (Krajči et al. 2017) can be found as the supplementary material from https://doi.org/10.1002/2017WR020445. All training data in this study was processed from these sources. The subsequent data supporting this study are available from the authors and can be obtained by submitting a direct request.

APPENDIX

Threshold Constraint Layers

a. Defining Threshold Constraint Layers

Since ReLu(x) = max(x,0), we can re-express the minimum and maximum functions in general as

\[ \max(x, y) = y + \text{ReLu}(x - y) = \text{ReLu}(y) - \text{ReLu}(-y) + \text{ReLu}(x - y) = \max(y, x), \quad (A1) \]

\[ \min(x, y) = y - \text{ReLu}(y - x) = \text{ReLu}(y) - \text{ReLu}(-y) - \text{ReLu}(y - x) = \min(y, x). \quad (A2) \]

Then for any model output p and any construction f that serves to threshold p, the threshold max(f, p) or min(f, p) can be explicitly implemented with a single depth-3 fixed-weight layer containing no biases acting on input \([p, f]^T\) with ReLu activation, followed by an accumulation
with no activation:

$$
\begin{bmatrix}
\pm 1 & 1 & -1
\end{bmatrix} \times \text{ReLU} \left( \begin{bmatrix}
\pm 1 & \mp 1 \\
0 & 1 \\
0 & -1
\end{bmatrix} \times \begin{bmatrix}
p \\
f
\end{bmatrix} \right) = A_{1\pm}^T \text{ReLU} \left( A_{2\pm}^T \begin{bmatrix}
p \\
f
\end{bmatrix} \right),
$$

(A3)

where taking the + indicates $\max(f, p)$ and taking the – indicates $\min(f, p)$, and the ReLu acts element-wise. The symmetry of the max and min functions also mean resonant structures (network structures outputting equivalent values but with different weights) also exist, Eq. A3 demonstrates one straightforward example.

Without additional knowledge of the sign of $p$ or $f$, both $+f$ and $-f$ (or $+p$ and $-p$, as the max and min functions are symmetric) need to be passed through the activated layer alongside the difference $p - f$ so the ReLu does not destroy any necessary information to calculate the threshold. However, if $f$ is always nonnegative (or nonpositive), the structure of the layer can be reduced, as there is no need to pass $-f$ (or $+f$ in the case of nonpositivity) as the ReLu will always evaluate to zero, so the depth of the fixed-weight layer can be reduced to two instead of three (this also holds if $p$ is nonnegative or nonpositive due to the symmetry of the max and min functions, so any additional knowledge of the sign of $f$ or $p$ permits a reduction in computational complexity by implementing the most reduced structural form). If the threshold always obeys $f \geq C$ or $f \leq C$ for some nonzero constant $C$, this reduction may still occur by including a bias term alongside $A_{2\pm}$ and $A_{1\pm}$ (the same holds for $p \geq C$ or $p \leq C$). Fig. A1a shows the generalized structure for such a one-sided threshold constraint function $f$ on the predictive model given in 2b.

Likewise, for a simultaneous upper bound $f_+$ and lower bound $f_-$ on $p$ for any constructions $f_+, f_-$ satisfying $f_+ \geq f_-$, we have

$$
\max(\min(p, f_+), f_-) = \text{ReLU}(f_-) - \text{ReLU}(-f_-) + \text{ReLU}(\alpha),
$$

(A4)

where

$$
\alpha = \text{ReLU}(f_+) - \text{ReLU}(-f_+) - \text{ReLU}(f_-) + \text{ReLU}(-f_-) - \text{ReLU}(f_+ - p),
$$

(A5)
so the threshold can be explicitly implemented with a sequence of two fixed-weight layers containing no biases acting on input \([p, f_+, f_-]^{T}\), followed by an accumulation with no activation:

\[
\begin{bmatrix}
-1 & 1 & -1 & -1 & 1 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix} \times \text{ReLU}
\begin{bmatrix}
-1 & 1 & 0 \\
0 & 1 & 0 \\
0 & -1 & 0
\end{bmatrix}
\times
\begin{bmatrix}
[p] \\
f_+ \\
f_-
\end{bmatrix}
\]

(A6)

\[
\begin{bmatrix}
1 & 1 & -1 & -1 & -1 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0
\end{bmatrix} \times \text{ReLU}
\begin{bmatrix}
-1 & 1 & 0 \\
0 & 1 & 0 \\
0 & -1 & 0
\end{bmatrix}
\times
\begin{bmatrix}
[p] \\
f_+ \\
f_-
\end{bmatrix}
\]

(A7)

which takes advantage of the identity \(\text{ReLU} (\text{ReLU}(x)) = \text{ReLU}(x)\). Like the one-sided threshold example, many resonant structures exist, particularly so as \(\max(\min(p, f_+), f_-) = \min(\max(p, f_-), f_+)\) when \(f_+ \geq f_-\). Similarly, knowledge of the sign (or constant bounds, if bias terms are included) of any of \(f_+, f_-\) can permit a reduction in the depth of the corresponding layers by astute choice of weights. Fig. A1b shows the generalized structure for such a two-sided threshold constraint function \(f\) outputting \(f_+, f_-\) on the predictive model given in 2b.

These constraint structures are adaptable to any desirable functional constraint \(f\) of any input (even those independent of the predictive model inputs) as well as the output of the predictive model \(p\). Such constraints could be analytically chosen, or unknown and parameterized constraints can be “learned” through training on observational data, even simultaneously alongside a trained predictive model (for instance, a network for threshold prediction and a network for value prediction for entirely data-driven predictive modeling). Combinations of different functional forms are also permitted under this architectural choice. Another advantage over other constraint approaches, such as projecting outputs into a constrained space, is that the thresholds do not need to be constant or even known beforehand, and the model can explicitly predict boundary values instead of asymptotically close values.

Figure A1 depicts the threshold constraint layers enveloping the entire predictive model from 2b, but for network-based predictive models, such structures could be placed inside larger networks,
Fig. A1. For all graphics, input data are on the left, model prediction is on the right, and the grey five-sided structure represents the predictive network shown in Fig. 1. Specific knowledge about the function $f$ can permit further reduction of these general layers by neglecting particular orange (ReLu) accumulation nodes, and resonant structures exist given the symmetry of max, min. Black weights contain no biases, are not trained, and equal +1 or -1 depending on the constraint. a) General structure of any one-sided constraint (a max or a min) on the predictive structure. b) General structure of any two-sided constraint (an enforced range) on the predictive structure.

layered, or stacked as part of a larger predictive model. In the case where the inputs of $p$ are shared with $f$, each constraint can be implemented with only one skip connection. Constrained networks of this type can be equivalently expressed with Maxout networks (Goodfellow et al. 2013) or nested networks for a given constraint form, though maintaining a single-network form with only one skip connection results in faster training and a wide variety of expression in constraint forms.

References


