Active Learning of Deep Surrogates for PDEs

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Deep Learning for Simulation (simDL)

Active learning algorithm filters the data with higher uncertainty to explore

Surrogate models for partial-differential equations are widely used in the design of metamaterials to rapidly evaluate the behavior of composable components. However, the training cost of accurate surrogates by machine learning can rapidly in-crease with the number of variables. We present an active learning algorithm and apply it to train deep surrogates of Helmholtz's equation and linear elasticity in solid mechanics. For the two problems of interest, our algorithm reduces the number of simulations required compared to uniform random samples by more than an order of magnitude for a neural-network surrogate model and by four, respectively. Results show that the surrogate evaluation is faster than a direct solve by over two orders of magnitude and over five orders of magnitude, respectively.

Surrogate model

A predictive model and an uncertainty quantification model.

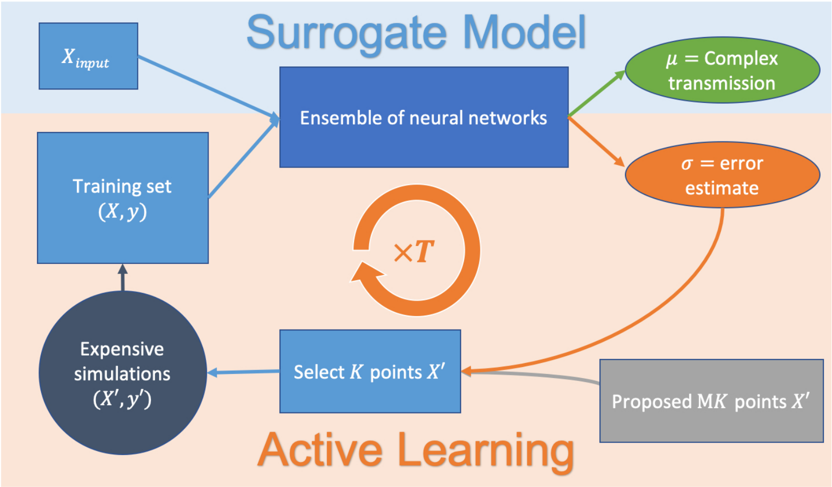
We iteratively rain a surrogate model and an uncertainty model concomitantly, to approximate a target physical response and measure the error of the model, respectively.

In the experiments below, the predictive and the uncertainty quantification model are combined into a heteroscedastic regression model. Where the prediction is the estimated mean, and the measure of error is the estimated variance.

$$-\sum_{\mathbf{p}} \log p_{\Theta_i}(y|\mathbf{p}) \propto \sum_{\mathbf{p}} \left[\log \sigma_i(\mathbf{p}) + \frac{(y(\mathbf{p}) - \mu_i(\mathbf{p}))^2}{2\sigma_i(\mathbf{p})^2}\right]$$

NB: the uncertainty quantification model only needs to be a monotonic increasing function of the true error of the model, because it is only used for ordering.
NB: The uncertainty quantification model of the heteroscedastic regression loses meaning interpolating regime, because the error becomes identically zero and does not take into account generalization error.

Active-learning algorithm

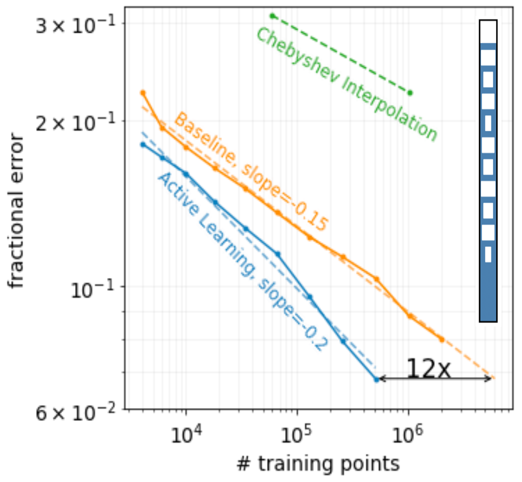


Input: n_{init}, T, M, K
Result: the surrogate model $\tilde{t}(\mathbf{p})$ (μ_* and σ_*)
$\mathcal{P}_0 = n_{\text{init}}$ points chosen from a random uniform distribution;
Solve PDE for each point in $\mathcal{P}_0$; `// expensive step`
Create the first iteration of the labeled training set $\mathcal{TS}_0$;
Train the ensemble $\tilde{t}^0(\mathbf{p})$ on $\mathcal{TS}_0$;
for i = $1{:}T$ **do**
  $\mathcal{R}_i$ = $M \times K$ points chosen from a random uniform distribution ;
  Compute the error measures $\sigma_*^{i-1}(\mathbf{p})$ using $\tilde{t}^{i-1}, \forall\, \mathbf{p} \in \mathcal{R}_i$; `// cheap step`
  $\mathcal{P}_i$ = select K points in $\mathcal{R}_i$ with the highest error measures σ_*^{i-1};
  Solve PDE for each points in $\mathcal{P}_i$ and get $t(\mathbf{p}), \forall\, \mathbf{p} \in \mathcal{P}_i$; `// expensive step`
  Augment the labeled training set with new labeled data $\mathcal{TS}_i$;
  Train the ensemble $\tilde{t}^i(\mathbf{p})$ on $\mathcal{TS}_i$ with warm start of $\tilde{t}^{i-1}$;
end

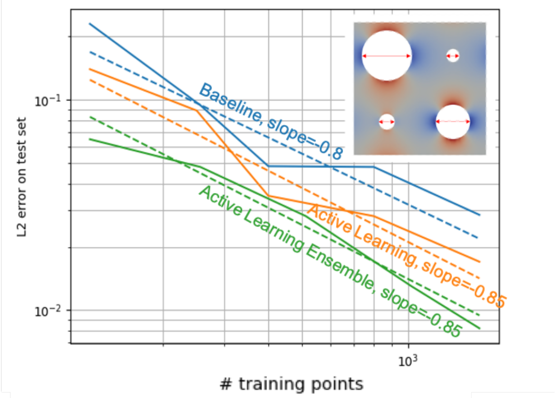
Typical M equals 4

Reduction of data need

Helmholtz's equation (speedup x100)



Linear elasticity (speedup x1.5e5)



References

Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. (2017) "Simple and scalable predic-tive uncertainty estimation using deep ensembles." In Proc. 31st Int. Conf. Advances in NeuralInformation Processing Systems, pp. 6402–6413. NIPS.

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