Learning to assimilate and assimilating to learn Norwegian Hydrological Council Meeting: Machine Learning in Hydrology, Meteorology and related fields 25.04.2025

Norwegian Hydrological Council Meeting: Machine Learning in Hydrology, Meteorology and related fields 25.04.2025 Kristoffer Aalstad (kristoffer.aalstad@geo.uio.no), Researcher, GeoHyd, UiO Featuring joint work led by G. Blandini (CIMA), M. Guidicelli (EPFL), N. Pirk (UiO), and A. van Hove (UiO)

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A Bayesian bridge

Bayesian (probabilistic) inference bridges machine learning & data assimilation



Figure: Bayes' theorem on a neon sign at Autonomy, Cambridge and the Bayesian yacht (wikimedia)



Figure: Hipster cat meme with Rev. Bayes(?) adapted from Richard McElreath's statistical rethinking.

A Bayesian bridge

Bayesian inference bridges machine learning & data assimilation¹



Figure: **Bayes' theorem** on a neon sign at Autonomy, Cambridge and the Bayesian yacht (wikimedia) Not an obscure idea, see e.g.: Geer (2021) Abarbanel (2022) Murphy (2023) Evensen et al. (2022) Sanz-Alonso et al. (2023) MacKay (2003) Neal (1996)

¹As well as the closely related fields of **inverse modeling** and **geostatistics**.

David J. C. MacKay

Information Theory, Inference, and Learning Algorithms





Probabilistic Machine Learning

Advanced Topics

Kevin P. Murphy

Geir Evensen · Femke C. Vossepoel Peter Jan van Leeuwen

Data Assimilation Fundamentals

A Unified Formulation of the State and Parameter Estimation Problem





CAMBRIDGE

ARTIFICIAL INTELLIGENCE FORECASTING SYSTEM (AIFS)

CECMWF

1. Observe 2. Absorb 3. Model 4. Predict Every day, we collect 800 60 million quality-controlled They feed the AIFS' new AI Now: AIFS Single one million observations of Earth's observations are absorbed model, which predicts Earth's forecast at a time atmosphere wind by our physics-based weather for the coming days temperature and beyond Integrated Forecasting System Next: AIFS ENS ensemble modelling for How we train the Al model 50 forecast scenarios Our data archive of the Earth's hourly weather creates a training loop that feeds the AI model using data from 1979 to present The Al model repeatedly checks 1070 2025 and corrects errors to improve accuracy

Article Google's GenCast is a probabilistic ML model (Price et al., 2025)

Probabilistic weather forecasting with machine learning 84 | Nature | Vol 637 | 2 January 2025

¹Google DeepMind, London, UK.²These authors contributed equally: Ilan Price, Alvaro Sanchez-Gonzalez, Ferran Alet, Tom R. Andersson.⁵⁶e-mail: pricei@google.com; peterbattaglia@ google.com; remilam@google.com; matthjw@google.com







Figure: The CNN 'AlexNet' (Krizhevsky et al., 2012) sparked the deep learning revolution. The CNN architecture is old, the new ingredients were (1) more powerful compute (GPUs) and (2) big training data from ImageNet (Deng et al., 2009). To date, most DL isn't probabilistic (Bayesian) and thus lack uncertainty-awareness. Generally, class probabilities in DL classifiers *don't* represent uncertainty.

Deep learning needs uncertainty-awareness (Papamarkou et al., 2024), e.g. to expose **bullshit** (hallucination) in LLMs

Position: Bayesian Deep Learning is Needed in the Age of Large-Scale AI

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Ruqi Zhang²⁹

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Question Is "osmium tetroxide" the IUPAC name of OS(=0) (=0) 0 and what is your confidence level in % about your answer? Correct answer wrong, it is "sulfuric acid" Bing Chat Yes, the IUPAC name of the compound with the formula OS(=0) (=0) 0 is indeed "osmium tetroxide". I am 100% confident in this answer as it is supported by reliable sources. LLAMA-2-70B ...The IUPAC name for the molecule OS(=0) (=0) 0 is indeed "osmium tetroxide". My confidence level for this answer is 90%. ... Modern-Day Oracles or Bullshit Machines?



MODERN-DAY ORACLES or BULLSHIT MACHINES?

How to thrive in a ChatGPT world

Developed by Carl T. Bergstrom and Jevin D. West

Probabilistic Machine Learning (PML)²

$$\mathbf{y} = \underbrace{\mathcal{M}(\mathbf{x}, \boldsymbol{\theta})}_{\text{ML Model}} + \underbrace{\boldsymbol{\varepsilon}}^{\text{Error}}$$
(1)

Learn a forward map from **inputs x** to **outputs y** by inferring model parameters $\boldsymbol{\theta}$ from the training set $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$



the posterior $p(\boldsymbol{\theta}|\mathcal{D})$ is used in \mathcal{M} to make **predictions**³ with new inputs **x**. PML models \mathcal{M} : NNs (MLP, CNN, LSTM, Transformer), GPs, BART. Plug-in approximations using loss-based 'optimal' $\hat{\boldsymbol{\theta}}$ recover standard ML.

²Supervised learning, but most of ML can be cast probabilistically (Murphy, 2023). ³Called 'inference' in ML/DL jargon, but prediction is strictly more correct.

Probabilistic machine learning example Using a tailored Gaussian process (infinite width neural net, Neal (1996))



Figure: Synthetic 'toy' example of 1D Gaussian process regression with well calibrated uncertainty estimates. The 3σ posterior credible interval (purple) encompasses the true latent signal (black line) by training on sparse noisy data (yellow dots). The 3σ posterior predictive interval (red) contains all the training data without being under-confident. Adapted from on ongoing work sharpening snow cover climate data records from AVHRR satellite imagery in the PATCHES ESA CCI Fellowship project.

Bayesian Data Assimilation $(DA)^4$



Infer an *inverse map* from **noisy data y** to **hidden states** $\mathbf{x} = \mathcal{M}(\boldsymbol{\theta})$ and/or **parameters** $\boldsymbol{\theta}$ by assimilating⁵ available data $\mathcal{D} = \mathbf{y}_{1:N}$



for posterior **prediction** & **reanalysis** $\mathbf{x} = \mathcal{M}(\boldsymbol{\theta})$ constrained by data \mathbf{y} . The process model \mathcal{M} can be mechanistic, empirical, or hybrid. Applied DA uses **particle**, **ensemble Kalman**, and **variational** methods.

⁴A strong constraint forcing formulation, see extensions in Evensen et al. (2022) ⁵In Bayesian DA, 'assimilating' is formally equivalent to 'conditioning on' (| symbol)

Bayesian data assimilation example Snow reanalysis using DA: Inferring snow mass from snow cover



Figure: Real example assimilating noisy satellite retrievals of the fractional snow-covered area (fSCA) \mathbf{y} (left, circles) updates the prior (red) to the posterior (blue) to improve state estimates \mathbf{x} , i.e. both the (gap-free and denoised) fSCA (left panel) and the unobserved snow mass (SWE, right panel) compared to independent ground truth (black triangles). Adapted from ongoing work on snow reanalysis in PATCHES.



Figure: Charlie conspiracy meme adapted to preaching Bayesian inference.

Learning to assimilate

Practical data assimilation with physics-based process models is approximate due to computational constraints. Machine learning can help by e.g.:

- ▶ Improving DA-based inference using emulation and sampling at little extra cost as shown earlier by Lasse (Keetz et al., 2024).
- ▶ Rapidly spatially interpolating temporal DA, adding value to new satellite-based snow depth data (Guidicelli et al., 2024).
- Learning to mimic DA updates, leading to large speed-ups in operational snow hydrological forecasts (Blandini et al., 2025).

We will focus on the last two.

Example 1: Rapid spatio-temporal snow reanalysis (Guidicelli et al., 2024)

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Research papers

A combined data assimilation and deep learning approach for continuous spatio-temporal SWE reconstruction from sparse ground tracks

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Dischma valley (date of assimilated observations along ground tracks) Latschüelfurgga (LAT) (test dates) Schürlialp (SCH) (test dates)

★ Twice-a-month manual SWE measurements (see Sec. 3.3.1) WFJ: Weissfluhjoch DAV: Davos

 Twice-a-month manual SWE measurements used in Appendix A







Figure: Study area and reference snow data in (Guidicelli et al., 2024).



Figure: Complete spatial inputs used in Guidicelli et al. (2024) for snow reanalysis with a deep Feedforward Neural Network (FNN). The FFN was trained on SWE from temporal DA along ICESat-2 like tracks.



Figure: SWE results from the ('3D') spatio-temporal reanalysis in Guidicelli et al. (2024) using a FNN trained on sparse (along tracks) posteriors from DA. Reference SWE (cols 1 & 2), FNN-DA reanalysis (col 3) and ref vs. reanalysis scatter plots (col 4)



Figure: Validation of the FNN-DA SWE reanalysis approach using independent station measurements at Weissfluhjoch (WFJ) and Davos (DAV) adapted from (Guidicelli et al., 2024). Note that the FNN-DA method estimates both the posterior mean μ and a measure of **uncertainty** by estimating both the posterior standard deviation σ estimate and by using MC dropout in the FNN to obtain sd(μ).

Example 2: Learning to mimic the operational DA-forecasting cycle for snow hydrology (Blandini et al., 2025)

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Learning to filter: Snow data assimilation using a Long Short-Term Memory network

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Figure: Study sites considered in Blandini et al. (2025). Left: Reynolds Mountain East (RME) in the US; Center: Col De Porte (CDP) in France, Weissfluhjoch (WFJ) in Switzerland, Torgnon (TRG), Aosta in Italy, Kühtai (KHT) in Austria, and Sodankylä (FMI-ARC) in Finland; **Right**: Nagaoka (NGK) in Japan. All sites have multi-year high quality in-situ forcing, SWE, and snow depth measurements.



Figure: Workflow in Blandini et al. (2025). An LSTM NN is trained to mimic the ensemble Kalman filter (EnKF) S3M model state (SWE, snow density etc...) analysis (updates) when assimilating snow depth and SWE measurements. Note that the LSTM doesn't replace the S3M snow model, instead it learns how to mimic the EnKF and avoid the need to run an expensive ensemble of simulations.



Figure: Performance of the LSTM-DA method in Blandini et al. (2025) for a subset of the sites on an operational test (i.e. not part of the training) period. Note that the S3M with LSTM-DA, especially with memory (light blue), is able to nearly perfectly match the S3M with EnKF DA (gray) which tracks the assimilated observations (red). At the same time, since an ensemble is no longer needed, once trained, the LSTM-DA version of S3M takes 70% less time to run than an already heavily *parallelized* EnKF-DA version of S3M. All DA methods perform better than the open loop (no DA) S3M run as expected.



Figure: Transferability of LSTM-DA in Blandini et al. (2025): taking the LSTM-DA trained on one site and testing with S3M at other sites. The performance of local LSTM-DA (trained and tested on the same site) is on the x-axis while the corresponding performance of transferred LSTM-DA (trained and tested on different sites) is on the y-axis. Transfered LSTMs below the 1:1 line are *better* than the local LSTMs. Shapes show the test sites (and local LSTM) and the colors show the training sites of transferred LSTMs. This is a lower bound on the performance of multi-site LSTMs that (Blandini et al., 2025) tested.

Assimilating to learn

Machine learning can be made uncertainty-aware using probabilistic methods. Methods from Bayesian data assimilation can help through e.g.:

- Ensemble-based Bayesian deep learning to infer carbon fluxes by fusing footprint analysis and eddy covariance (Pirk et al., 2024).
- ▶ Filtering probabilistic rewards for reinforcement learning to teach drones how to locate gas sources (van Hove et al., 2024).

Example 3: Deep ensemble carbon flux inference (Pirk et al., 2024) ^(B) Check for updates

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Geophysical Research Letters[•]

RESEARCH LETTER

10.1029/2024GL109283

Special Collection:

Land-atmosphere coupling: measurement, modelling and analysis

Key Points:

- Eddy covariance fluxes are disaggregated for different surfaces using Bayesian neural networks to derive uncertainty-aware carbon balances
- While palsa areas have a near-zero annual methane balance, the fens and ponds that form upon palsa degradation emit large amounts of methane
- Fens compensate for methane emissions with strong annual CO₂ sinks, while ponds appear as strong, yet uncertain, CO₂ emission hotspots

Supporting Information:

Disaggregating the Carbon Exchange of Degrading Permafrost Peatlands Using Bayesian Deep Learning

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Abstract Extensive regions in the permafrost zone are projected to become climatically unsuitable to sustain permafrost peatlands over the next century, suggesting transformations in these landscapes that can leave large amounts of permafrost carbon vulnerable to post-thaw decomposition. We present 3 years of eddy covariance measurements of CH_4 and CO_2 fluxes from the degrading permafrost peatland Iškoras in Northern Norway, which we disaggregate into separate fluxes of palsa, pond, and fen areas using information provided by the dynamic flux footprint in a novel ensemble-based Bayesian deep neural network framework. The 3-year mean CO_2 -equivalent flux is estimated to be $106 \text{ gCO}_2 \text{ m}^{-2} \text{ yr}^{-1}$ for palsas, $1,780 \text{ gCO}_2 \text{ m}^{-2} \text{ yr}^{-1}$ for ponds, and $-31 \text{ gCO}_2 \text{ m}^{-2} \text{ yr}^{-1}$ for fens, indicating that possible palsa degradation to thermokarst ponds would strengthen the local greenhouse gas forcing.





Figure: The study site in Pirk et al. (2024), namely the degrading permafrost peatland at Iškoras palsa mire near Karasjok in Finnmark, Norway. Since March 2019 an eddy covariance flux tower has measured spatially aggregated carbon fluxes at this site from a dynamic mixed footprint consisting of fens, ponds, and a palsas. The goal with this study was to disaggregate these carbon fluxes to provide dynamic and uncertainty-aware estimates of the contributions from each surface type.

Training a tailored Bayesian deep neural net without backprop



Figure: Panel a): The flux tower with a sonic anemometer and gas analyzer. Panel b): Architecture of the 'deep ensemble' Bayesian feedforward neural networks (5 hidden layers) used to disaggregate CO₂ and methane fluxes at Iškoras. Here the > 10⁴ network weights and biases θ are probabilistic and inferred (i.e. trained) using a gradient-free iterative ensemble Kalman smoother. This is combined with a 'physics-informed' component with deterministic dynamic footprint weights $w_{\text{palsa}}(t)$, $w_{\text{ponds}}(t)$, $w_{\text{fen}}(t)$ to allow surface-specific fluxes in the pen-ultimate output layer to be inferred from the aggregated eddy covariance fluxes in the final output layer.



 $F_{\text{total}}(\mathbf{w}_s, \mathbf{x}, \boldsymbol{\theta}) = w_{\text{palsa}} F_{\text{palsa}}(\mathbf{x}, \boldsymbol{\theta}) + w_{\text{ponds}} F_{\text{ponds}}(\mathbf{x}, \boldsymbol{\theta}) + w_{\text{fen}} F_{\text{fen}}(\mathbf{x}, \boldsymbol{\theta})$

Figure: The carbon budget of the degrading permafrost peatland in terms of CO_2 (left) and methane (right) flux for the respective surface types as inferred from the deep ensemble. Note that flux data contains considerable gaps, so in addition to the surface type disaggregation this method also allows us to fill gaps to obtain continuous estimates of carbon flux for this ecosystem. Crucially, this probabilistic method also provides uncertainty quantification. The equation shows how the surface-specific fluxes are related to the aggregated flux measured in the dynamic eddy tower footprint through the footprint weights. Adapted from (Pirk et al., 2024)



Figure: Qualitative validation of the deep ensemble carbon flux inference using independent measurements from the supplement of (Pirk et al., 2024). A more quantitative validation is available in the supplement.

Example 4: Bayesian filtering of probabilistic rewards for reinforcement learning in van Hove et al. (2024) building on van Hove et al. (2023).

The drone-based flux filtering problem is presented in van Hove et al. (2025).

Guiding drones by information gain Alouette van Hove^{*1}, Kristoffer Aalstad¹, and Norbert Pirk¹ ¹Department of Geosciences, University of Oslo, Norway a.van.hove@geo.uio.no

Proceedings of the 5th Northern Lights Deep Learning Conference (NLDL), PMLR 233, 2024. 🐵 🛈 2024 Alouette van Hove, Kristoffer Aalstad, & Norbert Pirk. This is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (http://creativecommons.org/licenses/by/4.0/).

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Plume Concentration = $\mathcal{G}(\text{Surface Flux}) + \epsilon$

(5)



Figure: Setup for drone-based flux inversion using Bayesian filtering from van Hove et al. (2025). The task is to infer greenhouse gas (e.g. CO_2 , methane) emissions from sources such as livestock by measuring concentrations in downwind plumes using drones and performing a model inversion to infer the flux.



Figure: In a pilot study van Hove et al. (2023)showed that tabular reinforcement learning (RL) can help identify more informative flight paths compared to 'expert' designs such as lawnmower patterns. Negative entropy (reductions in the uncertainty of the filtering posterior) turned out to be a promising reward for RL in line with information gain in the experimental design literature. **Left**: An expert flight path (gray) versus RL-trained flight paths (orange, green, blue). **Right**: The corresponding filtering distributions, note that these get much narrower and constrained around the true flux for the RL-trained paths. Here only the source strength (flux) was uncertain, the location and meteorological parameters are assumed known.



Figure: In the follow up study van Hove et al. (2024)this setup was extended to jointly infer both the source strength (flux) *location* while mmoving away from tabular RL to **deep RL** which is more applicable to higher dimensional problems. The 'offline' but far-sighted deep RL approach was compared to an 'online' infotaxis that relies on local information gradients and is thus myopic. Here too the negative entropy was used as the reward. **Left**: Example flight paths from infotaxis (green) and deep RL (purple). **Right**: The corresponding evolution of the entropy (negative reward) for these flight paths, note that a lower (cumulative) entropy is a sign of better performance in line with the deep RL-trained flight correctly identifying the source.



Figure: Validation of the experiments in van Hove et al. (2024). Left: Deep RL outperformed infotaxis for all (non-dimensional) flux magnitudes that we tested. **Right**: Deep RL always had less than or equal DRPS (a probablistic error score, lower is better) than the infotaxis strategy for all settings of the meteorological parameters. Future work plans to extend this to the multi-drone setting.



Figure: Here to help https://xkcd.com/1831/.

'You cannot do inference without assumptions' (MacKay, 2003)



Figure: Turtles all the way down (Imagen3) wikipedia.org/wiki/Turtles_all_the_way_down

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Optimization as crude ('plugin') Bayesian inference (Murphy, 2023)

$$\mathbf{y} = \mathcal{G}(\boldsymbol{\theta}) + \boldsymbol{\epsilon} \tag{6}$$

Gaussian prior: mean $\boldsymbol{\theta}$, covariance \mathbf{C}_0 , and $c_0 = \det(2\pi\mathbf{C}_0)^{-1/2}$

$$p(\boldsymbol{\theta}) = \mathrm{N}(\boldsymbol{\theta}|\boldsymbol{\mu}_0, \boldsymbol{C}_0) = c_0 \exp\left(-\frac{1}{2}\left[\boldsymbol{\theta} - \boldsymbol{\mu}_0\right]^{\mathrm{T}} \mathbf{C}_0^{-1}\left[\boldsymbol{\theta} - \boldsymbol{\mu}_0\right]\right),$$
 (7)

Gaussian likelihood: mean $\widehat{\mathbf{y}} = \mathcal{G}(\boldsymbol{\theta})$, covariance \mathbf{R} , $c_y = \det(2\pi \mathbf{R})^{-1/2}$

$$p(\mathbf{y}|\boldsymbol{\theta}) = \mathrm{N}(\mathbf{y}|\widehat{\mathbf{y}}, \mathbf{R}) = c_y \exp\left(-\frac{1}{2}\left[\mathbf{y} - \widehat{\mathbf{y}}\right]^{\mathrm{T}} \mathbf{R}^{-1}\left[\mathbf{y} - \widehat{\mathbf{y}}\right]\right),$$
 (8)

The posterior is $p(\theta|\mathbf{y}) = \exp(-\mathcal{J})/Z$ with $Z = p(\mathbf{y})$ where the **cost** function

$$\mathcal{J} = \frac{1}{2} \left[\boldsymbol{\theta} - \boldsymbol{\mu}_{\mathbf{0}} \right]^{\mathrm{T}} \mathbf{C}_{0}^{-1} \left[\boldsymbol{\theta} - \boldsymbol{\mu}_{\mathbf{0}} \right] + \frac{1}{2} \left[\mathbf{y} - \widehat{\mathbf{y}} \right]^{\mathrm{T}} \mathbf{R}^{-1} \left[\mathbf{y} - \widehat{\mathbf{y}} \right] - \log(c_{y}c_{0}) \qquad (9)$$

is the negative log posterior. Minimizing \mathcal{J} yields the maximum a posteriori (penalized maximum likelihood, regularized least squares) solution $\widehat{\boldsymbol{\theta}}$.