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Rank Histograms Estimators for Multi-Level Data Assimilation

Florian Beiser^{1,2,*}

Kjetil Olsen Lye¹

Håvard Heitlo Holm¹

Jo Eidsvik²

¹ SINTEF Digital, Norway

² Norwegian University of Science and Technology, Norway

* florian.beiser@sintef.no





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Motivation: Search-and-rescue at sea



Photo: Tom Kausanrød, Redningsselskapet

- Time-critical definition of search areas
 - Drift trajectories based on a simplified ocean model
 - Refined predictions by data assimilation
- Ensemble methods
 - Forecast together with associated uncertainty
 - EnKF approach for data assimilation
- Multi-level methods
 - Hierarchy of grid resolutions
 - Improving computational efficiency

Rank Histograms Estimators for Multi-Level Data Assimilation

1. Multi-Level Methods
 - Introduction of the basics
2. Rank Histograms
 - Overview of classical rank histograms
 - Multi-level estimation
3. Application
 - Multi-level data assimilation for simplified ocean model



Multi-Level Methods

Motivation

Uncertainty quantification

- Established tool
- Lower computational cost than single-level Monte Carlo at same accuracy

Multi-level data assimilation

- Recent efforts
- New challenges

Saving computational costs



ML-UQ

ML-DA

Multi-Level Methods


Ensemble

Hierarchy of grids with $N_x^0 < \dots < N_x^L$

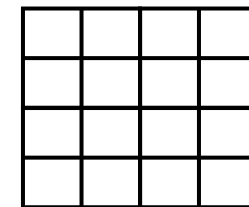
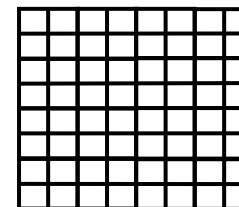
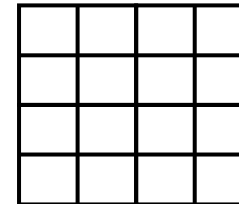
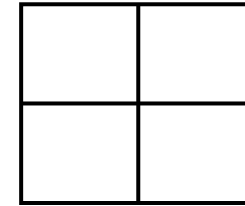
- Coarsest level

$$(x_n^0)_{n=1}^{N^0}$$

- Finer levels

$$(x_n^{l+}, x_n^{l-})_{n=1}^{N^l}$$


Same stochastic realisation
on consecutive grids



Multi-Level Methods

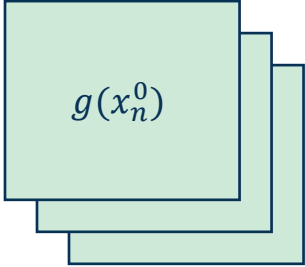
Estimator

- Smooth function g
- N^0, \dots, N^L optimally chosen for quantity of interest

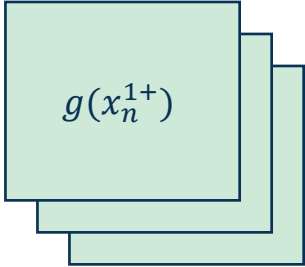
Multi-Level Estimator

$$\mathbb{E}[g(x^L)]$$

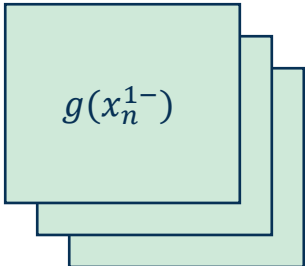
$$\approx \frac{1}{N^0} \sum_{n=1}^{N^0} g(x_n^0) + \sum_{l=1}^L \left(\frac{1}{N^l} \sum_{n=1}^{N^l} g(x_n^{l+}) - g(x_n^{l-}) \right)$$

$$\frac{1}{N^0} \sum_{n=1}^{N^0} g(x_n^0)$$


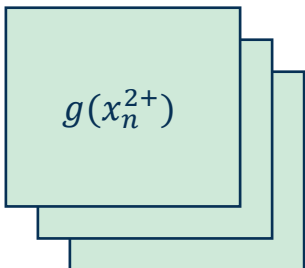
+

$$\left(\frac{1}{N^1} \sum_{n=1}^{N^1} g(x_n^{1+}) - g(x_n^{1-}) \right)$$


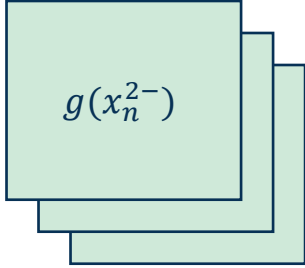
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+

$$\left(\frac{1}{N^2} \sum_{n=1}^{N^2} g(x_n^{2+}) - g(x_n^{2-}) \right)$$


-



Multi-Level Methods

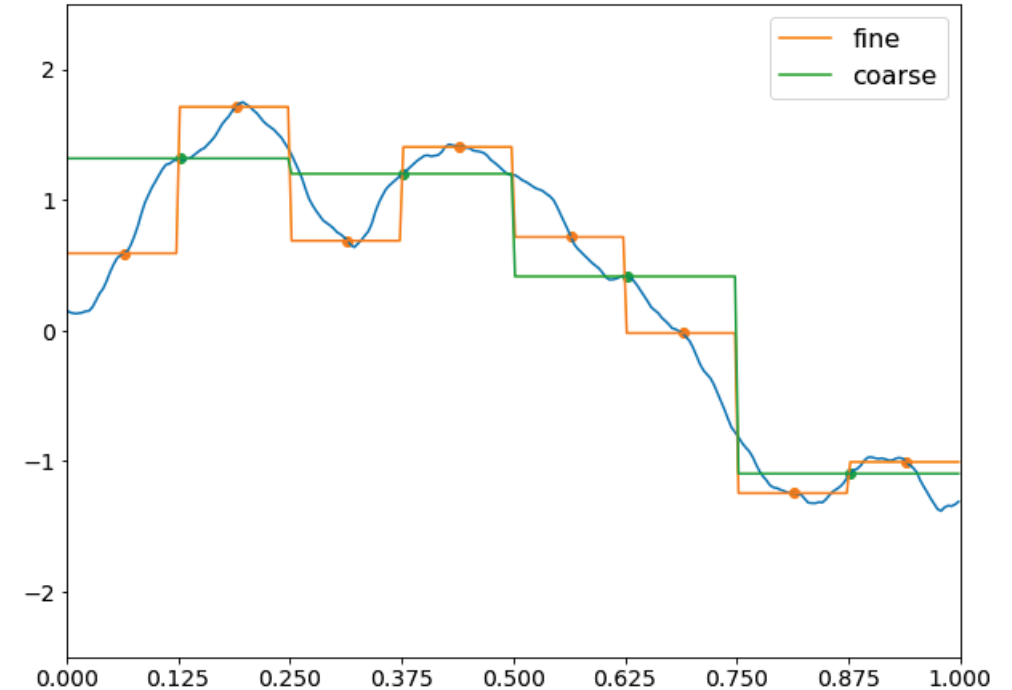
Gaussian Process

Example on interval $[0,1]$

$$x \sim \mathcal{N}(0, \mathbf{Q})$$

with Matern-like covariance matrix \mathbf{Q}

- Levels $l = 0, \dots, L$
- Values from 2^{4+l} equidistant points

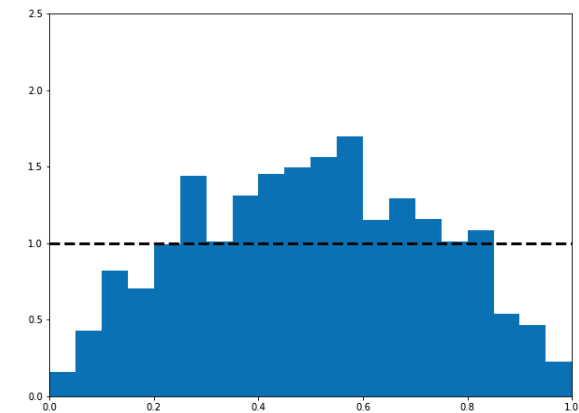
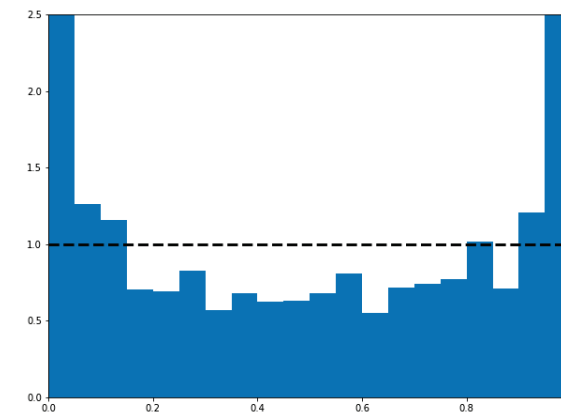
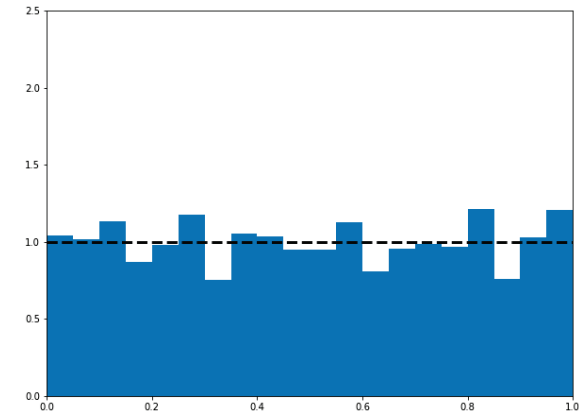
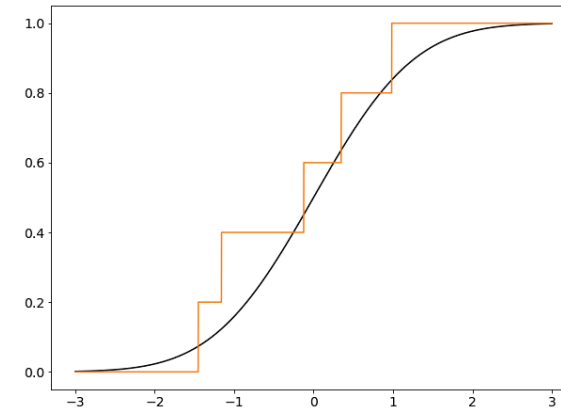


Rank Histograms *Overview*

- Assessing "right" spread of ensemble
 - Different skill scores suggested
 - Rank histograms common in practice
- Rank Histograms
 - Tracking rank of truth in sorted ensemble
 - Repeating experiment multiple times
- What rank of true y mathematically is:

$$\text{rank}(y) = P(X \leq y)$$

$$= \mathbb{E}[1_{(-\infty, y]}(X)]$$



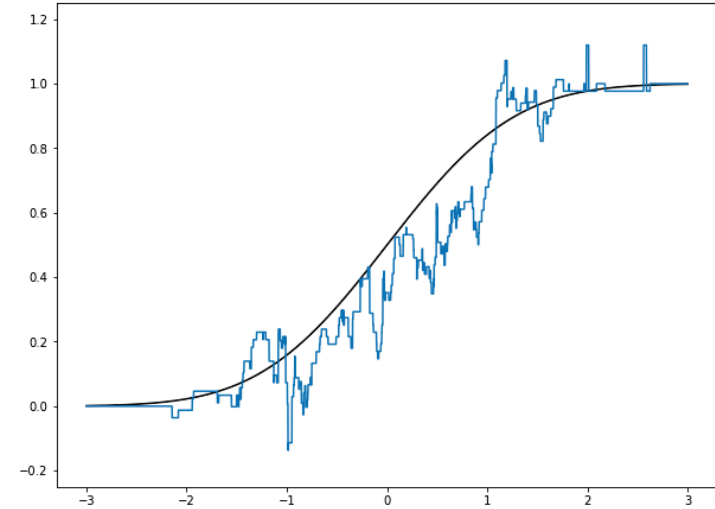
Rank Histograms Overview

Representative ensemble size 43, 43, 28, 15, 7

$$\frac{1}{N^0} \sum_{n=1}^{N^0} 1_{(-\infty, y]}(x_n^0) + \sum_{l=1}^L \left(\frac{1}{N^l} \sum_{n=1}^{N^l} 1_{(-\infty, y]}(x_n^{l+}) - 1_{(-\infty, y]}(x_n^{l-}) \right)$$

Multi-level comes at a price:

- (Fixed) ensemble size is not good for approximation of indicator function
- Direct evaluation of expected value does not yield feasible CDF!



Empirical CDF

- Direct evaluation of expected value
- Evaluation of expected value with smoothing
- Maximum entropy with polynomial basis

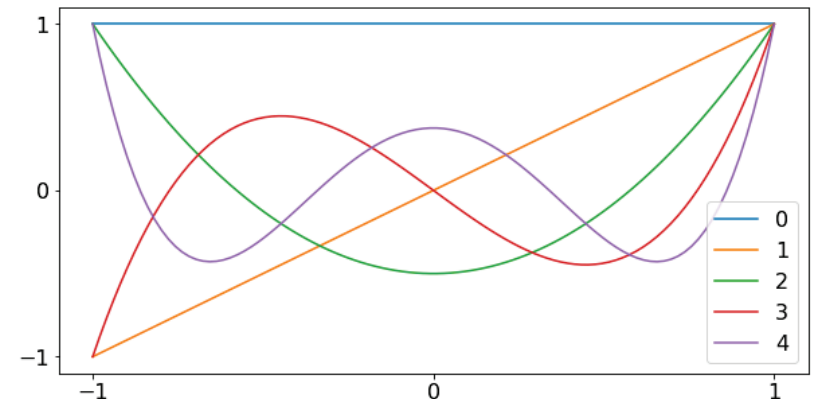
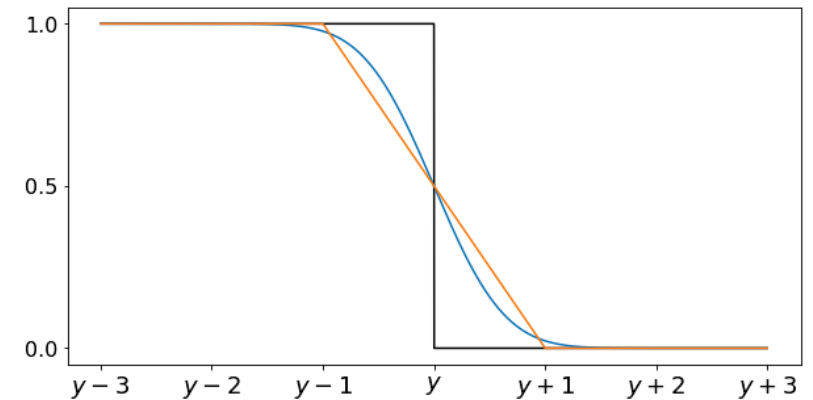
Rank Histograms Overview

Smoothing of $1_{(-\infty, y]}$

- Kernel with bandwidth ρ
 - Gaussian
 - Piecewise linear

Maximum entropy

- For set of basis functions $\phi_0, \dots, \phi_{N-1}$
- PDF approximation by $p = \exp(\sum_{i=0}^{N-1} \lambda_i \phi_i)$
- Maximising Shannon entropy
- Constraints $\mathbb{E}[\phi_i] = \int \phi_i p \, dx$



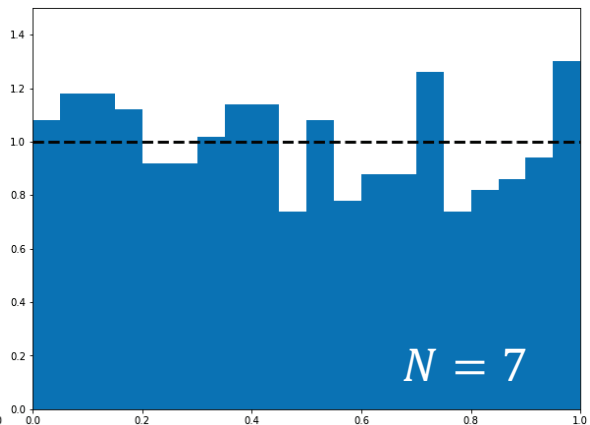
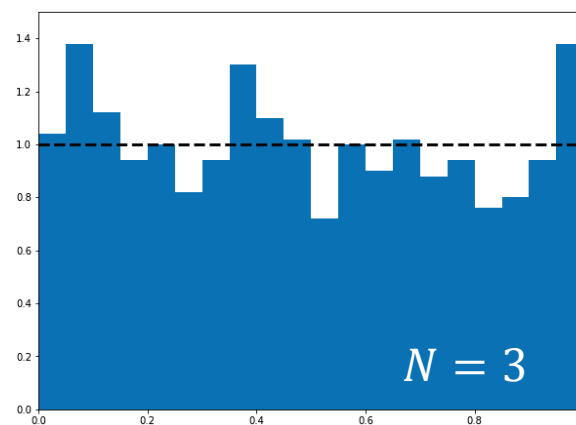
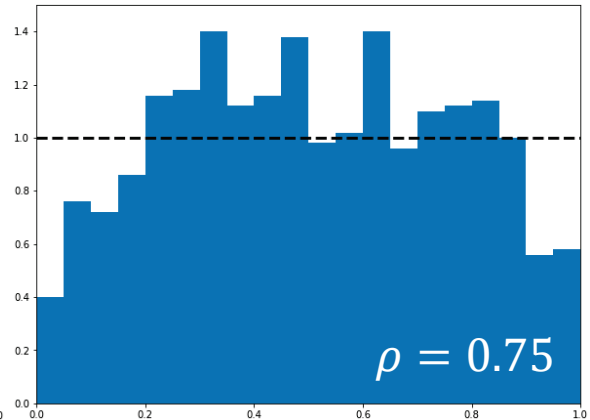
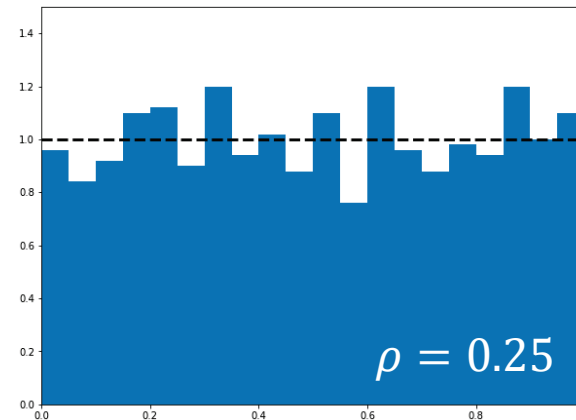
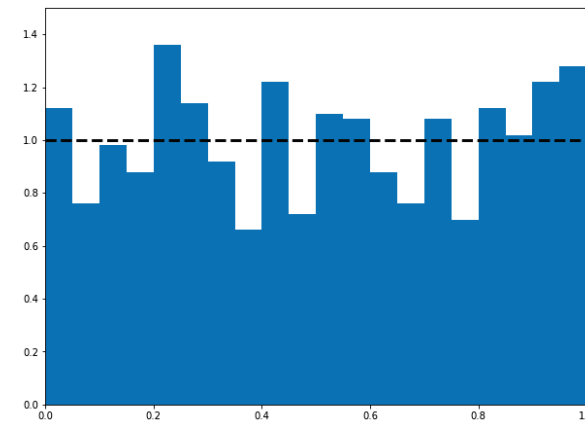


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Rank Histograms *Overview*

- *Single-level* ensemble with 50 members
- Truth and ensemble from same distribution

1. Direct evaluation
2. Smoothing
3. Maximum entropy





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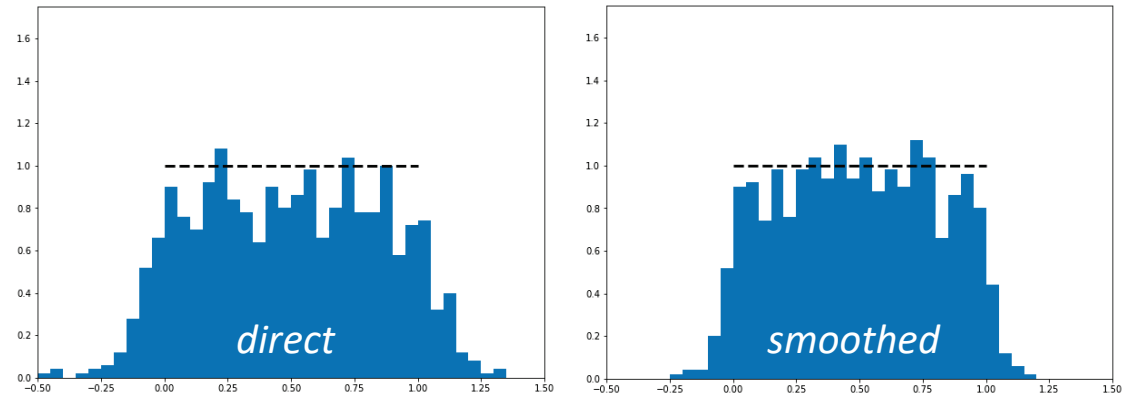
Rank Histograms

Multi-Level

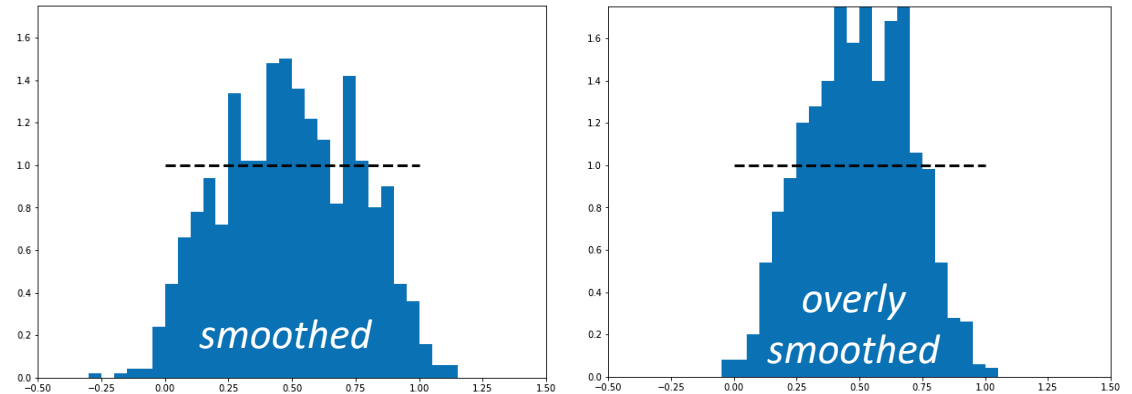
- Multi-level ensemble
- Smoothing:
The finer level, the bigger bandwidth
- Case with enhanced variance

- Always applicable
- Choice of bandwidth must not affect interpretability

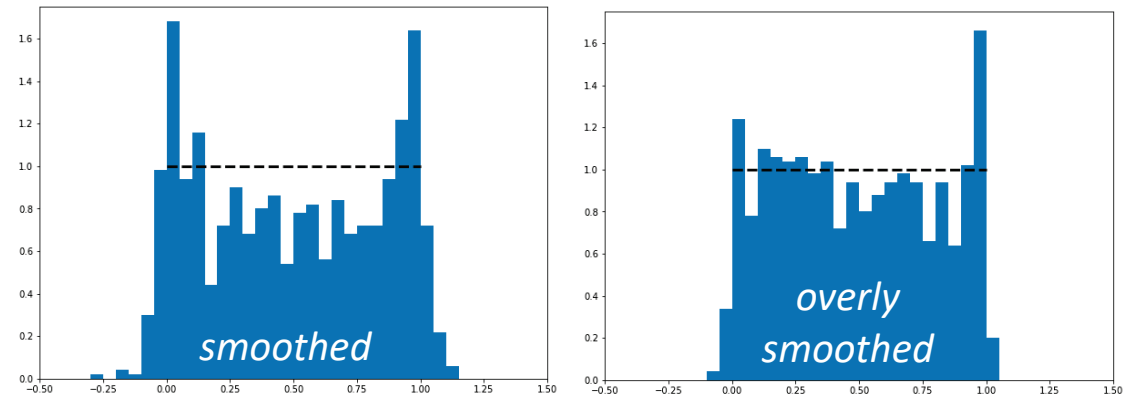
True variance = ensemble variance



True variance < ensemble variance



True variance > ensemble variance





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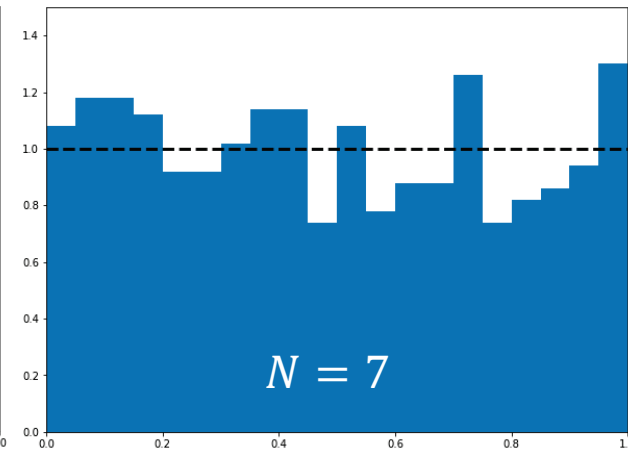
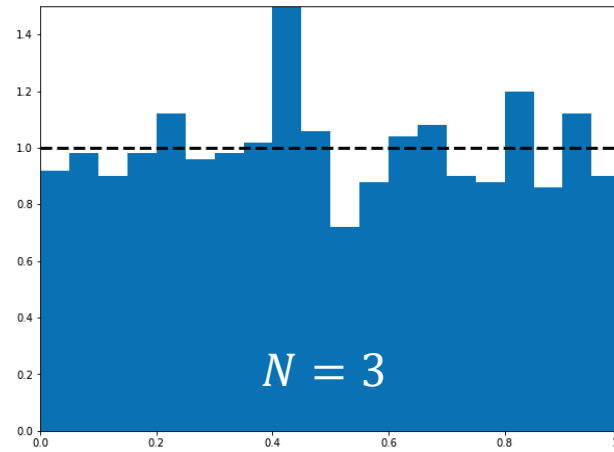
Rank Histograms

Multi-Level

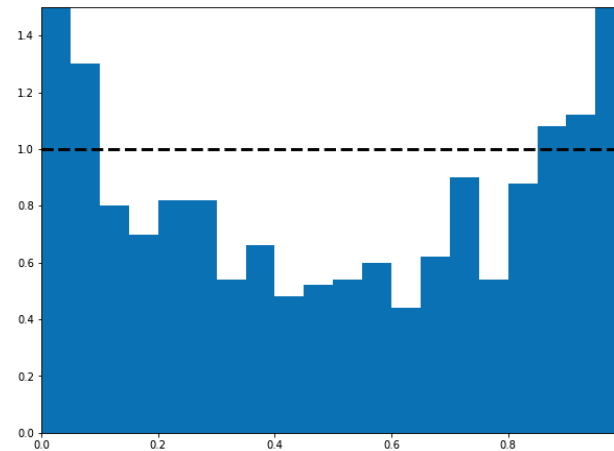
- Multi-level ensemble
- Maximum entropy with Legendre basis

- Few parameters
- Ranks are always $[0,1]$
- Sensitive to estimation quality of $\mathbb{E}[\phi_i]$
- Convergence issues with high variance

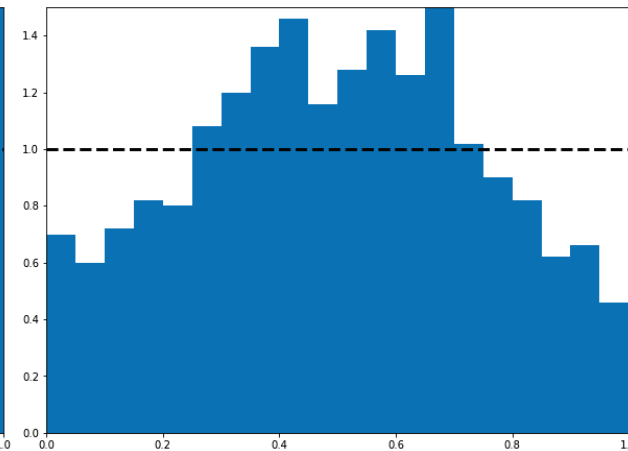
True variance = ensemble variance



True variance
>
ensemble variance



True variance
<
ensemble variance



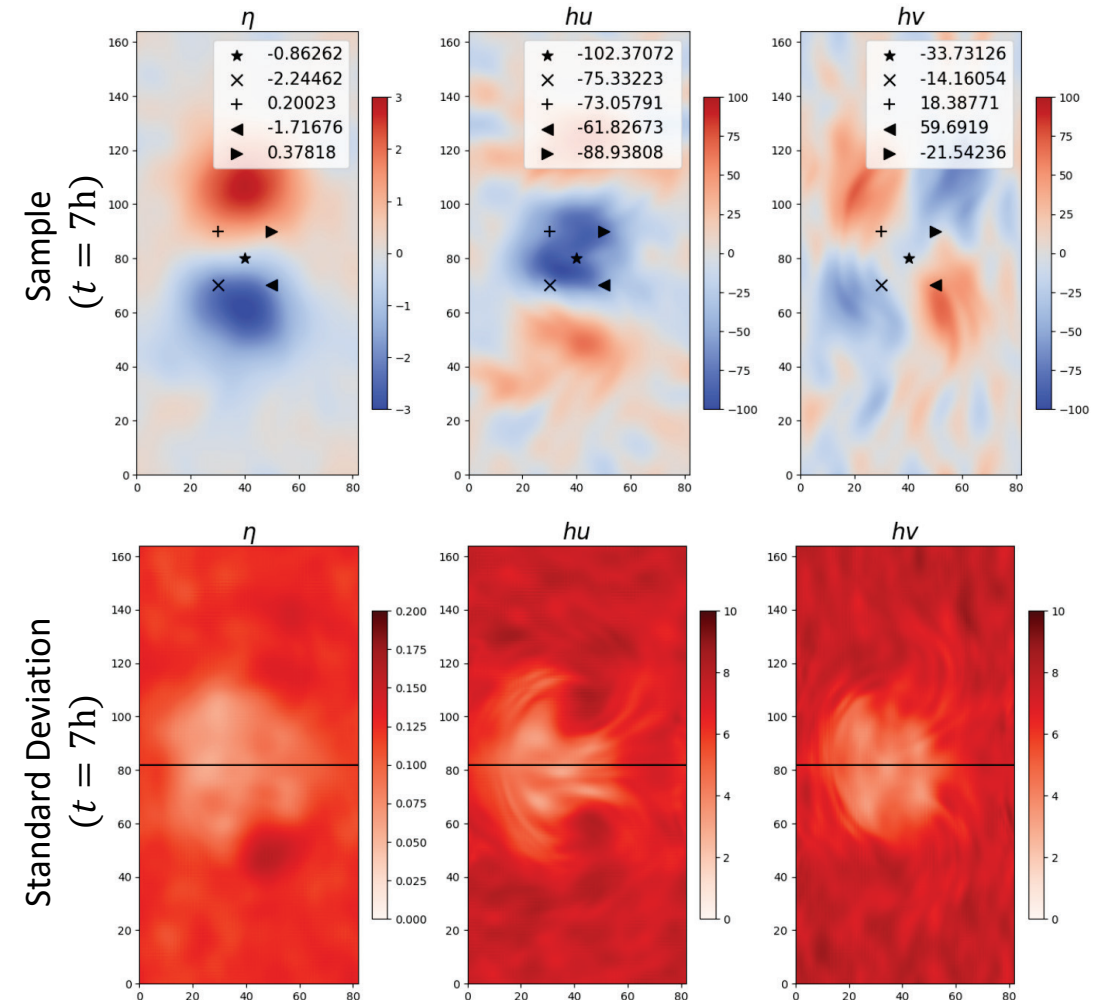


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Application

MLEnKF for simplified ocean model

- Rotational shallow-water model
 - h : water column. η : deviation from equilibrium
 - u, v : velocities in x, y -direction
 - Additive Gaussian error
- Data assimilation with MLEnKF*
 - Ensemble size 313, 84, 26, 6
 - Sparse observations in center
 - 6h simulation with DA every 15min
 - 1h forecast
- Rank histograms
 - Observing locations along horizontal line



* Chernov, Hoel, Law, Nobile, Tempone: *Multilevel Ensemble Kalman filtering for spatio-temporal processes*.

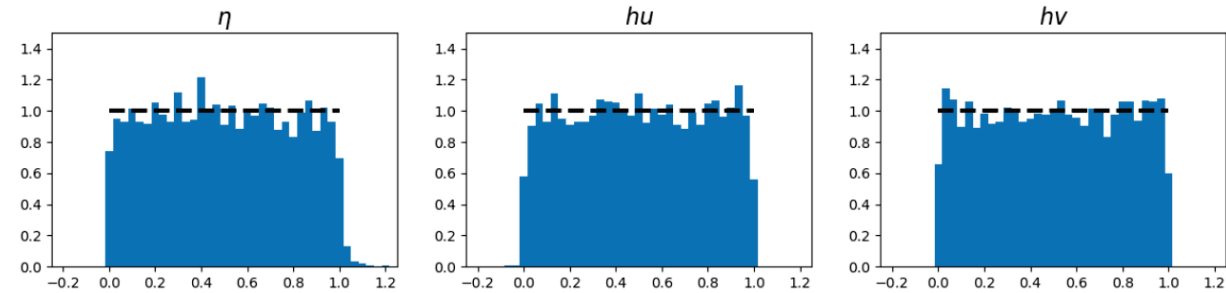
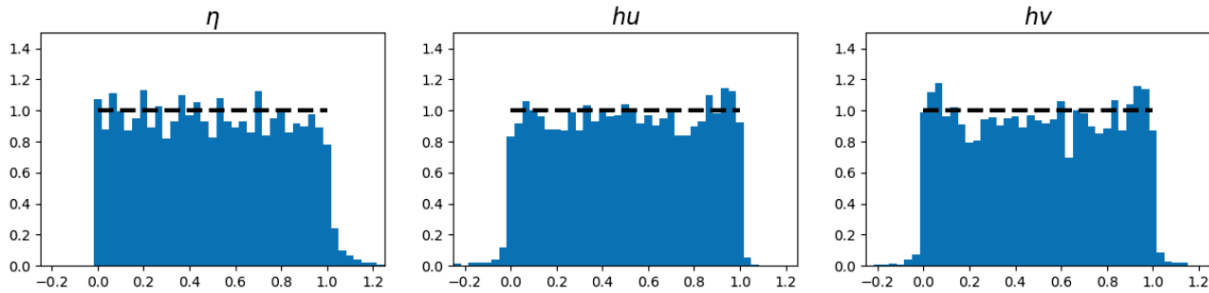


Application

MLEnKF for simplified ocean model

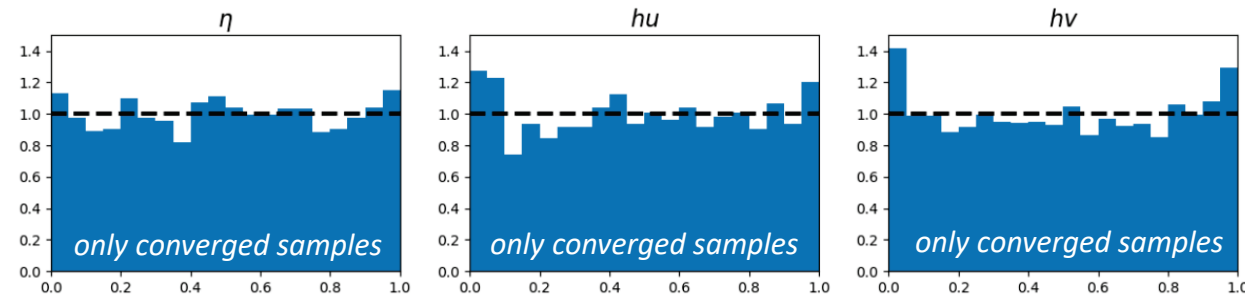
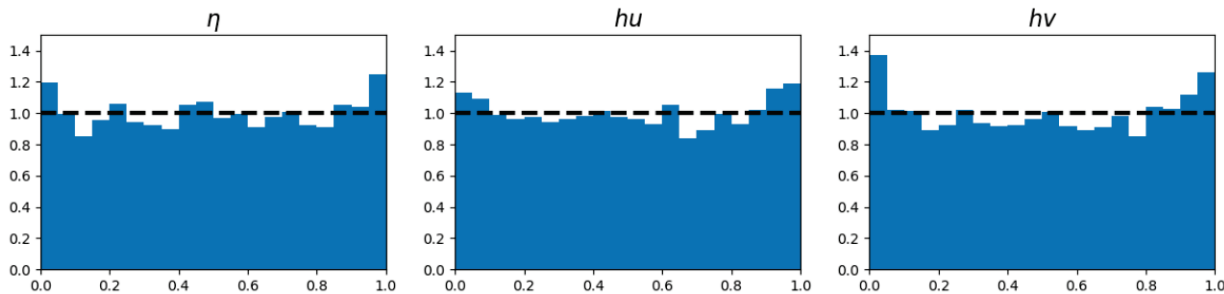
Direct evaluation

Smoothing with increasing bandwidth



Maximum entropy ($N = 3$)

Maximum entropy ($N = 5$)





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Closing Remarks

- Multi-level ensembles interesting approach for the future
- Still open question how to evaluate ensemble spread
- For small multi-level ensemble size, the direct evaluation of ranks might be infeasible
- Three approaches to calculate rank histograms discussed
- Multi-level rank histograms provide tool to evaluate spread in multi-level DA



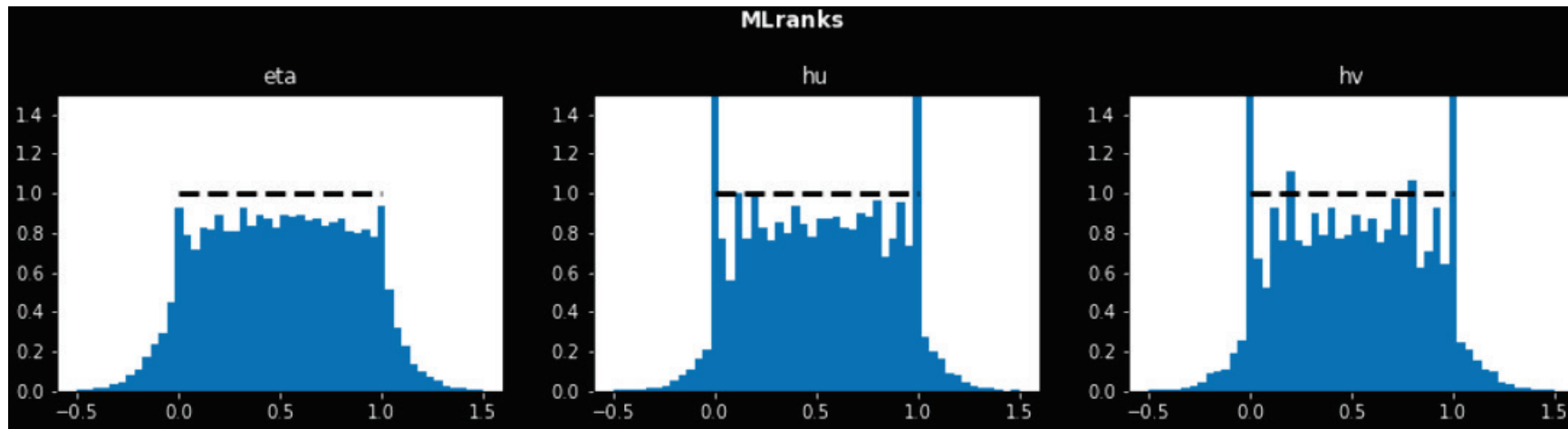
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Technology for a
better society



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SWE rank histograms (initial prior)





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Ranks per level (GP, different run)

