da.rs: Data-Assimilation in Rust

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December 19, 2017

This document describes a mathematical concept of the data assimilation, and how it is implemented on this crate.

1 Probability Distribution

1.1 Gaussian

A Normal distribution $\mathcal{N}(\mu, \Sigma)$, where μ denotes the center and Σ denotes covariance matrix, is implemented in two forms:

- Mixture (m-) representation `dars::gaussian::M`
- Exponential (e-) representation `dars::gaussian::E`

Each representations are defined in the `dars::gaussian` module. Mixture representation is simple: it contains `center` and covariance matrix `cov`.

2 Ensemble Kalman Filter

The PDF is represented by an ensemble $\{x_t^i\}$ $(i = 1, 2, \dots, K)$. Each of the ensemble member x_t^i is also called "particle" and an element of the state space $\mathbb{R}^N$. We consider a finite dimensional state space to establish a library for data-assimilation. Ensemble $\{x_t^i\}$ is represented by a wrapper of two-dimensional array `dars::ensemble::Ensemble` defined in `dars::ensemble`.

2.1 Ensemble-Transform Kalman Filter (ETKF)

Ensemble Space E_t is defined for an ensemble at time t:

$$E_t = \left\{ \sum_i w_i x_t^i \middle| \sum_i w_i = 1 \right\} \tag{1}$$

This is an Affine sub-space of the state space $\mathbb{R}^N$. Ensemble Transform Kalman Filter (ETKF) models the Bayesian update due to observations by an Affine transformation on E_t. Since an Affine transformation (A, b) can be applied both to ensemble and Gaussian, we can find a transformation corresponds to a Bayesian update for a Gaussian. However, the number of Affine transformations corresponding to a Bayesian for a Gaussian update is not one due to the symmetry of the Gaussian distribution. Symmetric square-root algorithm (a.k.a. square-root filter) is often used to reduce this redundancy.

1. Take a m-Projection $\left\{x_t^i\right\} \mapsto \mathcal{N}(\mu_t^b, \Sigma_t^b)$
2. Bayesian update $\mathcal{N}(\mu_t^b, \Sigma_t^b) \mapsto \mathcal{N}(\mu_t^a, \Sigma_t^a)$
3. Find an Affine transform (A, b) s.t. $\mu_t^a = A\mu_t^b + b$, $\Sigma_t^a = A\Sigma_t^b A^T$
4. Apply the Affine transformation to the ensemble $\left\{x_t^i\right\} \mapsto \left\{Ax_t^i + b\right\}$

For simple calculation, a weight space $S \subset \mathbb{R}^K$ is used to be introduced:

$$S = \left\{ w \in \mathbb{R}^K \,\middle|\, \sum_i w_i = 1 \right\} \tag{2}$$

A injection $\phi_t : S \to E_t$ is an isomorphic linear transform:

$$\phi_t : S \ni w \mapsto \sum_i w_i x_t^i \in E_t, \tag{3}$$

and is represented by a matrix $\phi_t = (x_t^1 \cdots x_t^K)$. The inverse of this injection induces the m-projected Gaussian onto S, and it is represented by $\mathcal{N}(w_0, \Omega_0)$ where $w_0 = (1/K, \dots, 1/K)^T$ and $\Omega_0 = (I - Kw_0w_0^T)/(K-1)$. This can be regarded as a projected distribution of $\mathcal{N}(0, I/(K-1))$ on $\mathbb{R}^K$ using the projection $P_0 = I - Kw_0w_0^T : \mathbb{R}^K \to S$. Then the Bayesian updated PDF $p(w|y)$ on $\mathbb{R}^K$ is following[1]:

$$\begin{aligned} -2\ln p(w|y) &= \|P_0(w - w_0)\|^2 + \|y - H\phi_t P_0 w\|^2_{R^{-1}} + \text{const.} \qquad (4) \\ &= \|P_0(w - \tilde{w})\|^2_{\tilde{\Omega}_t^{-1}} + \text{const.}, \qquad (5) \end{aligned}$$

where H is the observation operator whose domain is extended onto $\mathbb{R}^K$ using the projection P_0, and[2].

$$\begin{aligned} \tilde{\Omega}_t^{-1} &= \frac{1}{K-1} I + Y_t^T R^{-1} Y_t \qquad (7) \\ \tilde{w} &= \tilde{\Omega}_t Y_t^T R^{-1}(y - Y_t w_0) \qquad (8) \\ Y_t &= H\phi_t P_0. \qquad (9) \end{aligned}$$

[1] $\|x\|_A^2$ denotes $x^T Ax$ for positive semi-definite symmetric matrix A

[2] Be sure that

$$\|P_0 w - \tilde{w}\|^2_{\tilde{\Omega}_t^{-1}} = \|P_0(w - \tilde{w})\|^2_{\tilde{\Omega}_t^{-1}} + \text{const.} \tag{6}$$

Once we obtain a Gaussian $\mathcal{N}(\tilde{w}, \tilde{\Omega}_t)$ on $\mathbb{R}^K$, we seek an Affine transformation (A, b) corresponding to the Bayesian update $\mathcal{N}(0, I/(K-1)) \mapsto \mathcal{N}(\tilde{w}, \tilde{\Omega}_t)$ and project it onto S. The correspondence condition of Affine transformation is following:

$$\tilde{w} = b \tag{10}$$

$$\tilde{\Omega}_t = \frac{1}{K-1} A A^T \tag{11}$$

The redundancy of the Affine transformation is represented this condition, and we use symmetric square root in ndarray-linalg crate $A = \sqrt[S]{(K-1)\tilde{\Omega}}$. Finally, it induces an Affine transformation $(\phi_t P_0 A, \phi_t P_0 b)$ on E_t.