Covariance Propagation in Data Assimilation: A Continuum Analysis of Advective Systems

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Motivation: Addressing Variance Loss in Data Assimilation

Data Assimilation as a Discrete Problem

Daley (1991), Kalnay (2003), Evensen (2009), etc.

$$\boldsymbol{P}_{k+1} = \boldsymbol{M}_{k+1,k} \left(\boldsymbol{M}_{k+1,k} \boldsymbol{P}_k\right)^T + \boldsymbol{Q}_k.$$

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Continuum Analysis of Covariance Propagation

Return to the continuum in an effort to uncover the underlying cause of variance loss in the propagation step.

Part I: Analyze the continuum covariance propagation and uncover a discontinuous change in dynamics,

Part II: Derive the dynamics approximated by numerical schemes along the covariance diagonal.

Part I:
Continuum Covariance Propagation

Part I: Generalized Advective Dynamics

Define $q = q(\boldsymbol{x}, t)$ for $\boldsymbol{x} \in S_r^2$ with q_0 stochastic with mean $\overline{q}_0$, $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{x}, t)$ the (deterministic) velocity field, and $b = b(\boldsymbol{x}, t)$ a (deterministic) scalar,

$$q_t + \boldsymbol{v} \cdot \boldsymbol{\nabla} q + bq = 0,$$

$$q(\boldsymbol{x}, t_0) = q_0(\boldsymbol{x}).$$

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Let $\mathbb{E}\{\cdot\}$ denote the expectation operator, and define the covariance $P = P(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \mathbb{E}\big\{\big[q(\boldsymbol{x}_1, t) - \overline{q(\boldsymbol{x}_1, t)}\big]\big[q(\boldsymbol{x}_2, t) - \overline{q(\boldsymbol{x}_2, t)}\big]\big\}$,

Continuum Covariance Evolution Equation

$$P_t + \boldsymbol{v}_1 \cdot \nabla_1 P + \boldsymbol{v}_2 \cdot \nabla_2 P + (b_1 + b_2)P = 0,$$

$$P(\boldsymbol{x}_1, \boldsymbol{x}_2, t_0) = P_0(\boldsymbol{x}_1, \boldsymbol{x}_2).$$

Part I: Dynamics Along the Hyperplane $x_1 = x_2$

$$(\mathcal{P}_t f)(\boldsymbol{x}_1) = \int_{S_r^2} P(\boldsymbol{x}_1, \boldsymbol{x}_2, t) f(\boldsymbol{x}_2) d\boldsymbol{x}_2, \;\; f \in L^2(S_r^2)$$

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↙

spatially correlated (continuous) q_0

$P_0(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sigma_0(\boldsymbol{x}_1) C_0(\boldsymbol{x}_1, \boldsymbol{x}_2) \sigma_0(\boldsymbol{x}_2)$

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Variance Equation

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spatially uncorrelated q_0

$$P_0(\mathbf{x}_1, \mathbf{x}_2) = P_0^c(\mathbf{x}_1) \delta(\mathbf{x}_1, \mathbf{x}_2)$$

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Continuous Spectrum Equation

$$P(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = P^c(\boldsymbol{x}_1, t) \delta(\boldsymbol{x}_1, \boldsymbol{x}_2)$$
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Part I: Variances Extracted from Full Rank Covariance Propagation

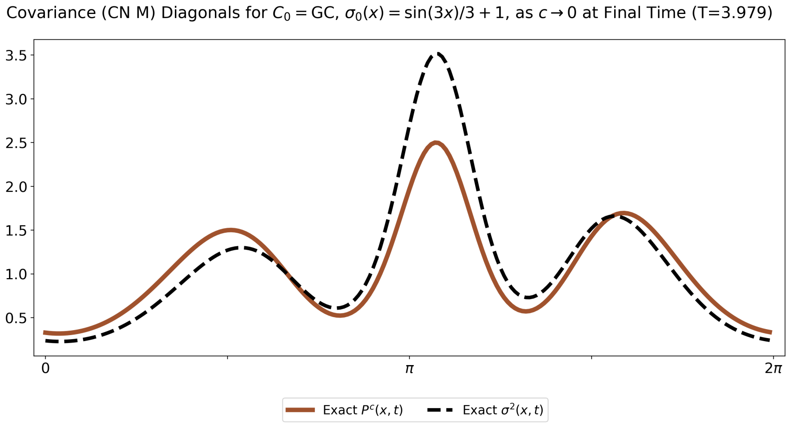


Figure 1: Exact solutions to the variance equation (σ^2, black dashed) and continuous spectrum equation (P^c, brown solid) at time T (slightly after a full period) for a spatially-varying initial condition. The state dynamics satisfy the continuity equation ($b = v_x$) with velocity $v(x) = \sin(x) + 2$.

The variance, σ^2 (black dashed), and continuous spectrum, P^c (brown solid), are distinct when the velocity field varies in space.

Part I: Variances Extracted from Full Rank Covariance Propagation

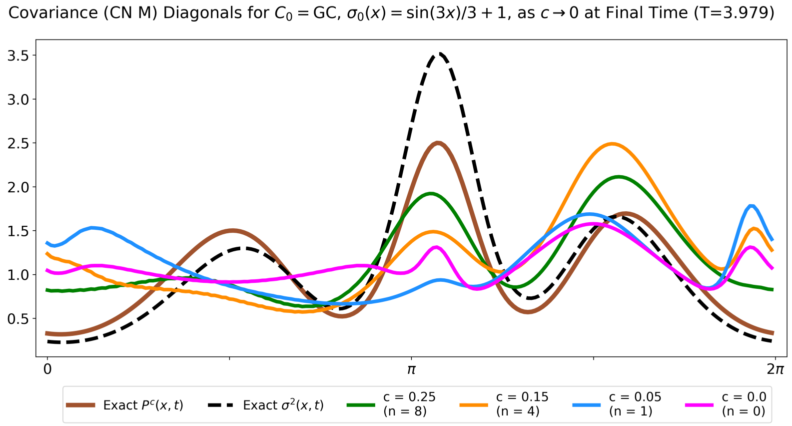


Figure 2: Diagonals extracted from covariances matrices propagated forward to time T (slightly after a full period) using the Crank-Nicolson finite difference scheme for covariances with different initial correlation lengths (linearly proportional to c in legend).

As correlation lengths shrink, the numerically propagated diagonals are approximating *something*, though it is unclear what is being approximated.

Part I: Concluding Thoughts, Insights, and Lingering Questions

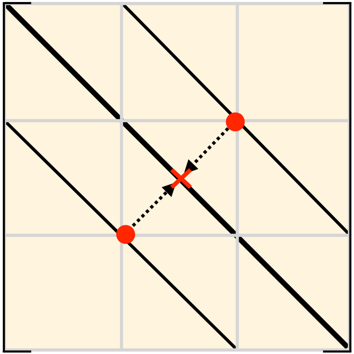
- **Key Insight:** The discontinuous change in the continuum dynamics causes problems when propagating covariance diagonals in discrete space.
- Both spurious loss and gain of variance are observed.
- What is $\boldsymbol{M}(\boldsymbol{M}\boldsymbol{P})^T$ trying to approximate along the covariance diagonal?

Part II:
Error Analysis of $M(MP)^T$

Part II: $M(MP)^T$ and the Covariance Diagonal

Covariance propagation,

$$\boldsymbol{P}_{k+1} = \boldsymbol{M}_{k+1,k}\left(\boldsymbol{M}_{k+1,k}\boldsymbol{P}_k\right)^T$$



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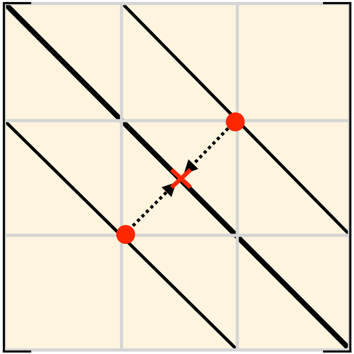

How does approximating the covariance diagonal with off-diagonal elements impact the dynamics being approximated *along* the diagonal?

Part II: Semi-Discretization for the Covariance Diagonal Propagation

Consider the generalized advection equation in *flux form* on the unit circle (S_1^1), $v > 0$,

$$q_t + (vq)_x + (b - v_x)q = 0$$

Part II: Semi-Discretization for the Covariance Diagonal Propagation

Consider the generalized advection equation in *flux form* on the unit circle (S_1^1), $v > 0$,

$$q_t + (vq)_x + (b - v_x)q = 0$$

Apply a *first-order upwind spatial discretization* for $x_i = i\Delta x$, $i = 1, 2, ..., N$, $\Delta x = \frac{2\pi}{N}$,

$$\frac{d}{dt}q_i(t) = \frac{1}{\Delta x}\left[v_{i-1}(t)q_{i-1}(t) - v_i(t)q_i(t)\right] - \left[b_i(t) - (v_x)_i(t)\right]q_i(t).$$

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Define $P_{i,j}(t) = \mathbb{E}\big\{[q_i(t) - \overline{q}_i(t)][q_j(t) - \overline{q}_j(t)]\big\}$ and take $i = j$,

$$\frac{d}{dt}P_{i,i}(t) = \frac{1}{\Delta x}\Big\{v_{i-1}(t)\big[P_{i-1,i}(t) + P_{i,i-1}(t)\big] - 2v_i(t)P_{i,i}(t)\Big\} - 2\big[b_i(t) - (v_x)_i(t)\big]P_{i,i}(t).$$

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Averaging across the diagonal to approximate $P_{i-1/2,i-1/2}(t)$

Part II: Approximated Dynamics Along the Covariance Diagonal

Variance Equation

$$\sigma^2_t = -\left(v\sigma^2\right)_x - \left(2b - v_x\right)\sigma^2$$

Continuous Spectrum Equation

$$P^c_t = -\left(vP^c\right)_x - \left(2b - 2v_x\right)P^c$$

Part II: Approximated Dynamics Along the Covariance Diagonal

Variance Equation

$$\sigma_t^2 = -\left(v\sigma^2\right)_x - \left(2b - v_x\right)\sigma^2$$

Continuous Spectrum Equation

$$P_t^c = -\left(vP^c\right)_x - \left(2b - 2v_x\right)P^c$$

First-Order Upwind:

$$\begin{aligned}\frac{d}{dt}P(x_i, x_i, t) = {} & -(vP)_x|_{x_1=x_2=x_i}\left[1 - \frac{\Delta x^2}{8L^2(x_i,t)}\right] - \left[2b(x_i,t) - 2v_x(x_i,t)\right]P(x_i,x_i,t) \\ & - v_x(x_i,t)P(x_i,x_i,t)\left[1 - \frac{\Delta x^2}{8L^2(x_i,t)}\right] - \frac{1}{\Delta x}\frac{\Delta x^2}{4L^2(x_i,t)}v(x_i,t)P(x_i,x_i,t) \\ & + \tilde{G}_u(x_i,t) + \tilde{H}_u(x_i,t).\end{aligned}$$

Part II: Approximated Dynamics for First- and Second-Order Schemes

First-Order Upwind:

$$\frac{d}{dt}P(x_i,x_i,t) = -(vP)_x|_{x_1=x_2=x_i}\left[1-\frac{\Delta x^2}{8L^2(x_i,t)}\right] - \left[2b(x_i,t)-2v_x(x_i,t)\right]P(x_i,x_i,t)$$
$$- v_x(x_i,t)P(x_i,x_i,t)\left[1-\frac{\Delta x^2}{8L^2(x_i,t)}\right] - \frac{1}{\Delta x}\frac{\Delta x^2}{4L^2(x_i,t)}v(x_i,t)P(x_i,x_i,t)$$
$$+ \tilde{G}_u(x_i,t) + \tilde{H}_u(x_i,t).$$

Second-Order Centered Difference:

$$\frac{d}{dt}P(x_i,x_i,t) = -(vP)_x|_{x_1=x_2=x_i}\left[1-\frac{\Delta x^2}{8L^2(x_i,t)}\right] - \left[2b(x_i,t)-2v_x(x_i,t)\right]P(x_i,x_i,t)$$
$$- v_x(x_i,t)P(x_i,x_i,t)\left[1-\frac{\Delta x^2}{8L^2(x_i,t)}\right]$$
$$+ \tilde{G}_c(x_i,t) + \tilde{H}_c(x_i,t)$$

Part II: Significance of $\Delta x^2/8L^2(x,t)$

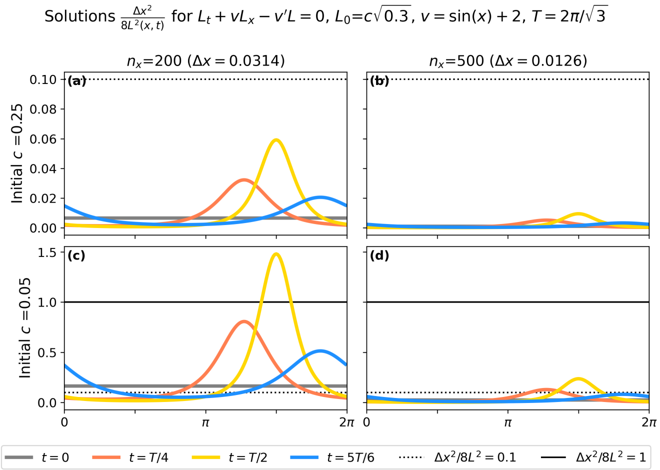


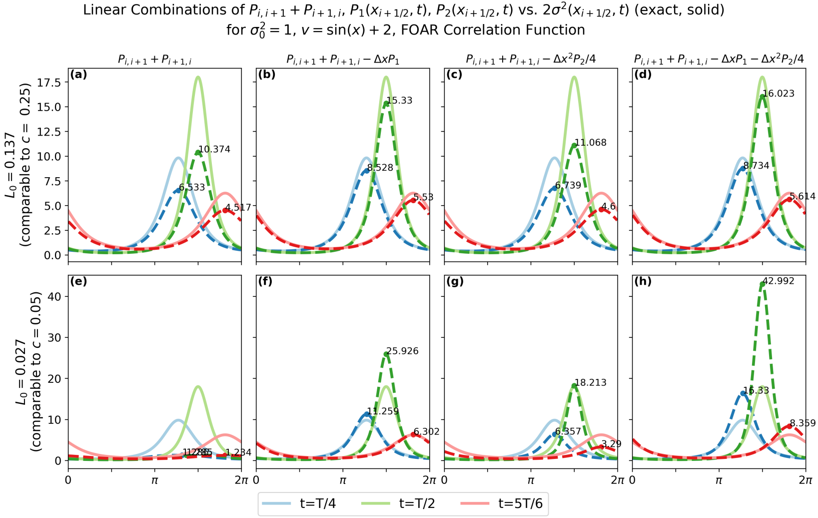
Figure 3: Time series snapshots of the ratio $\Delta x^2/8L^2(x,t)$ for different initial correlation lengths and grid lengths (uniform discretization of the unit circle).

Correlation lengths $L(x,t)$ satisfy

$$L_t + vL_x - v_x L = 0.$$

For the first-order upwind discretization, the term $-\frac{1}{\Delta x}\frac{\Delta x^2}{4L^2(x_i,t)} v(x_i,t) P(x_i,x_i,t)$ can become large even when $\frac{\Delta x^2}{8L^2(x_i,t)}$ is small.

Part II: Higher Order Average Approximations



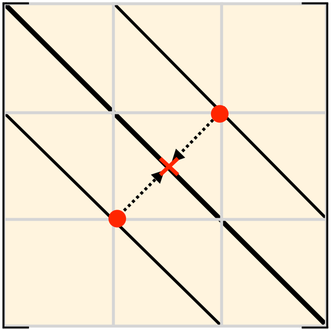
Higher order average approximations do not always result in better approximations of the covariance diagonal.

Figure 4: Time series snapshots of higher order average approximations (dashed) compared to the exact solution (solid).

Part II: Concluding Thoughts, Lingering Questions, and Further Investigation

- **Key Insight:** Approximating the diagonal with off-diagonal elements changes the dynamics approximated along the covariance diagonal.
- For advective systems, the approximated dynamics depend on ratio of the grid resolution to the correlation length, $\frac{\Delta x}{L}$.
- What does this suggest about covariance propagation practiced in current data assimilation schemes?

$$\boldsymbol{P}_{k+1} = \boldsymbol{M}_{k+1,k}(\boldsymbol{M}_{k+1,k}\boldsymbol{P}_k)^T$$



Acknowledgements and Questions

For more information or further discussion, contact Shay at **shay.gilpin@colorado.edu**

Relevant work:

Gilpin, Matsuo, and Cohn, (2022): *Continuum covariance propagation for understanding variance loss in advective systems*, SIAM/ASA JUQ.

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Extra Slides

Motivation Spurious Loss of Variance in 2D Transport Model

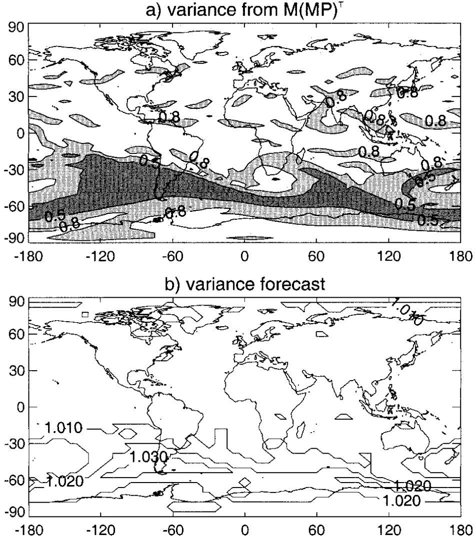

Figure 1 from Ménard et al. (2000), illustrating the variances $\sigma^2(\boldsymbol{x}, t)$ associated with the covariance $P(\boldsymbol{x}_1, \boldsymbol{x}_2, t)$ on an isentropic surface of Earth's atmosphere governed by

$$\boxed{P_t + \boldsymbol{v}_1 \cdot \boldsymbol{\nabla}_1 P + \boldsymbol{v}_2 \cdot \boldsymbol{\nabla}_2 P = 0.}$$

(a) variance extracted from the discrete covariance propagation $\boldsymbol{M}(\boldsymbol{MP})^T$, (b) variance obtained by solving the associated equation for the variance,

$$\boxed{\sigma_t^2 + \boldsymbol{v} \cdot \boldsymbol{\nabla} \sigma^2 = 0, \;\; \sigma_0^2 = 1.}$$

Motivation: Spurious Loss of Variance in 3D Transport Model

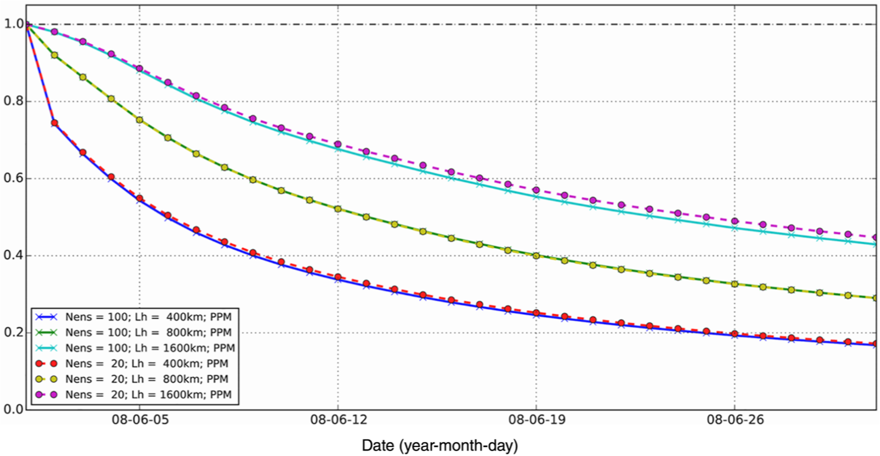

FIGURE 5 Total error variance evolution using ERA-Interim winds for different initial correlation length using 20 and 100 members

Figure 5: Figure 5 from Ménard et al. (2021) depicting the total error variance as a function of time for different ensemble experiments in a 3*D* chemical transport model (chemistry turned off, advection only).

Part I: The Hyperplane $x_1 = x_2$ is a Characteristic Surface

The characteristic equations for $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ both satisfy

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}(\boldsymbol{x}, t),$$
$$\boldsymbol{x}(t_0) = \boldsymbol{s},$$

where $\boldsymbol{x}_i = \boldsymbol{x}(t; \boldsymbol{s}_i)$ for the initial coordinate $\boldsymbol{s}_i$, $i = 1, 2$.

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If $\boldsymbol{s}_1 = \boldsymbol{s}_2$, then for $t \geq t_0$

$$\boldsymbol{x}_1 = \boldsymbol{x}(t; \boldsymbol{s}_1) = \boldsymbol{x}(t; \boldsymbol{s}_2) = \boldsymbol{x}_2,$$

solutions that start on the hyperplane $\boldsymbol{x}_1 = \boldsymbol{x}_2$ remain on this hyperplane for all time.

As a result, *there is a discontinuous change in covariance dynamics as initial correlation lengths tend to zero.*

Part I: The Fundamental Solution Operator

We can write solutions to the state equation as

$$q(\boldsymbol{x}, t) = (\boldsymbol{\mathcal{M}}_t q_0)(\boldsymbol{x}),$$

where $\boldsymbol{\mathcal{M}}_t \colon L^2(S_r^2) \mapsto L^2(S_r^2)$ is the *fundamental solution operator*

$$(\boldsymbol{\mathcal{M}}_t f)(\boldsymbol{x}) = \int_{S_r^2} M(\boldsymbol{x}, t; \boldsymbol{\xi}) f(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad f \in L^2(S_r^2),$$

whose kernel $M = M(\boldsymbol{x}, t; \boldsymbol{\xi})$ satisfies

$$M_t + \boldsymbol{v} \cdot \boldsymbol{\nabla} M + bM = 0,$$

$$M(\boldsymbol{x}, t_0; \boldsymbol{\xi}) = \delta(\boldsymbol{x}, \boldsymbol{\xi}).$$

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$$M_t + \boldsymbol{v} \cdot \boldsymbol{\nabla} M + bM = 0,$$
$$M(\boldsymbol{x}, t_0; \boldsymbol{\xi}) = \delta(\boldsymbol{x}, \boldsymbol{\xi}).$$

We can also define the *adjoint fundamental solution operator*, $\boldsymbol{\mathcal{M}}_t^* \colon L^2(S_r^2) \mapsto L^2(S_r^2)$, defined by

$$(\boldsymbol{\mathcal{M}}_t^* f, g)_2 = (f, \boldsymbol{\mathcal{M}}_t g)_2 \quad \forall f, g \in L^2(S_r^2),$$

which is also an integral operator,

$$(\boldsymbol{\mathcal{M}}_t^* f)(\boldsymbol{\xi}) = \int_{S_r^2} M^*(\boldsymbol{\xi}; \boldsymbol{x}, t) f(\boldsymbol{x}) d\boldsymbol{x}, \quad f \in L^2(S_r^2).$$

Part I: Continuum Covariance Propagation (Operator Formulation)

We can express the covariance $P(\boldsymbol{x}_1, \boldsymbol{x}_2, t)$ in terms of the kernels M and M^*,

$$P(\boldsymbol{x}_1, \boldsymbol{x}_2, t) = \int_{S_r^2} \int_{S_r^2} M(\boldsymbol{x}_1, t; \boldsymbol{\xi}_1) P_0(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) M^*(\boldsymbol{\xi}_2; \boldsymbol{x}_2, t) d\boldsymbol{\xi}_2 d\boldsymbol{\xi}_1,$$

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or simply

$$\boldsymbol{\mathcal{P}}_t = \boldsymbol{\mathcal{M}}_t \boldsymbol{\mathcal{P}}_0 \boldsymbol{\mathcal{M}}_t^*,$$

where $\boldsymbol{\mathcal{P}}_t \colon L^2(S_r^2) \mapsto L^2(S_r^2)$ is the *covariance operator*,

$$(\boldsymbol{\mathcal{P}}_t f)(\boldsymbol{x}_1) = \int_{S_r^2} P(\boldsymbol{x}_1, \boldsymbol{x}_2, t) f(\boldsymbol{x}_2) d\boldsymbol{x}_2, \quad f \in L^2(S_r^2),$$

where at $t = t_0$ we have

$$(\boldsymbol{\mathcal{P}}_0 f)(\boldsymbol{x}_1) = \int_{S_r^2} P_0(\boldsymbol{x}_1, \boldsymbol{x}_2) f(\boldsymbol{x}_2) d\boldsymbol{x}_2, \quad f \in L^2(S_r^2).$$

Part II: Expanding the Averaging Term

$$\frac{d}{dt}P_{i,i}(t) = \frac{1}{\Delta x}\Big\{v_{i-1}(t)\big[P_{i-1,i}(t) + P_{i,i-1}(t)\big] - 2v_i(t)P_{i,i}(t)\Big\} - 2\big[b_i(t) - (v_x)_i(t)\big]P_{i,i}(t).$$

The natural choice is to expand about the half-grid point $x_{i-1/2}, x_{i-1/2}$.

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$$P(x_{i-1}, x_i, t) + P(x_i, x_{i-1}, t) = 2P(x_{i-1/2}, x_{i-1/2}, t) + \left(\frac{\Delta x}{2}\right)^2 P_2(x_{i-1/2}, t) + \mathcal{O}(\Delta x^3).$$

$$P_2(x,t) = \left[\frac{\partial^2 P}{\partial x_1^2} - 2\frac{\partial^2 P}{\partial x_1 \partial x_2} + \frac{\partial^2 P}{\partial x_1^2}\right]_{x_1 = x_2 = x} = P(x,x,t)\log\big[P(x,x,t)\big]_{xx} - \underbrace{\frac{P(x,x,t)}{L^2(x,t)}}_{\text{correlation length}}$$

Part II: Semi-Discretization in Advection Form (Upwind)

Suppose we consider the state equation in advection form,

$$q_t + vq_x + bq = 0,$$

and discretize q_x using a first-order upwind scheme,

$$\frac{d}{dt}q_i(t) = \frac{v_i(t)}{\Delta x}\left[q_{i-1}(t) - q_i(t)\right] - b_i(t)q_i(t).$$

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The semi-discretization for the covariance diagonal is then,

$$\frac{d}{dt}P_{i,i}(t) = \frac{v_i(t)}{\Delta x}\Big\{\big[P_{i-1,i}(t) + P_{i,i-1}(t)\big] - 2P_{i,i}(t)\Big\} - 2b_i(t)P_{i,i}(t)$$

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The approximated dynamics (after expanding the averaging term) are

$$\frac{d}{dt}P(x_i,x_i,t) = -\,v(x_i,t)P_x(x_i,x_i,t)\left[1 - \frac{\Delta x^2}{8L^2(x_i,t)}\right] - 2b(x_i,t)P(x_i,x_i,t)$$
$$-\frac{1}{\Delta x}\frac{\Delta x^2}{4L^2(x_i,t)}v(x_i,t)P(x_i,x_i,t) + A_u(x_i,t) + B_u(x_i,t)$$