Observing Simulation System Expertiment (OSSE) for point-vortex models

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Point-vortex systems: vortex motion

Consider m point vortices in the plane whose the equations of motion of the $k-$th vortices are given by

$$\frac{dx_k}{dt} = -\frac{1}{2\pi}\sum_{\substack{j=1\\ j\neq k}}^{m} \kappa_j \frac{y_k - y_j}{(x_k - x_j)^2 + (y_k - y_j)^2}$$

$$\frac{dy_k}{dt} = \frac{1}{2\pi}\sum_{\substack{j=1\\ j\neq k}}^{m} \kappa_j \frac{x_k - x_j}{(x_k - x_j)^2 + (y_k - y_j)^2},$$

where κ_j denotes the vortex strength.

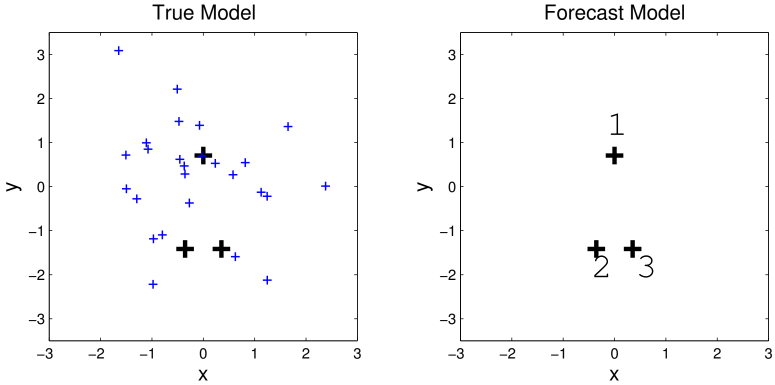
Point-vortex systems: tracer motion

The motion of passive tracers (denoted by (x, y) without any subscript) depends explicitly on time through the positions of vortices. The velocity filed of the passive tracers are given by

$$\frac{dx}{dt} = -\frac{1}{2\pi}\sum_{j=1}^{m}\kappa_j\frac{y_k - y_j}{(x_k - x_j)^2 + (y_k - y_j)^2}$$

$$\frac{dy}{dt} = \frac{1}{2\pi}\sum_{j=1}^{m}\kappa_j\frac{x_k - x_j}{(x_k - x_j)^2 + (y_k - y_j)^2}.$$

"True" and Forecast Models



Truth and Model Forecast

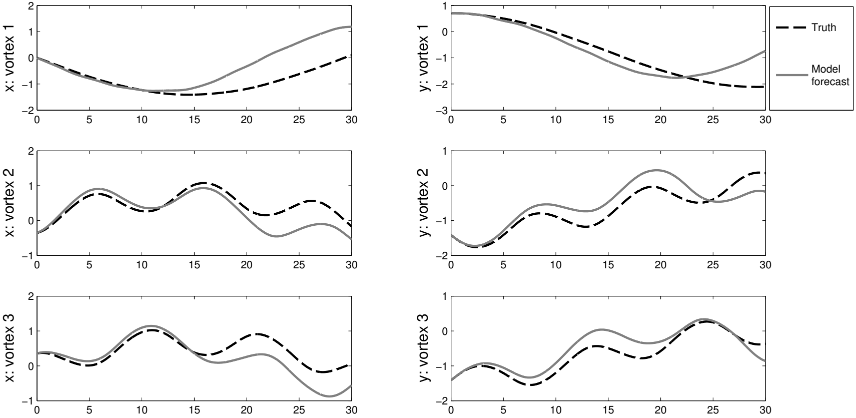


Figure: $\kappa_1 = \kappa_2 = \kappa_3 = 1$, $\kappa_j = 0.03$ for $j = 4, \ldots, 30$. The RMSEs for the three vortices are 0.64, 0.43 and 0.44, respectively.

Lagrangian Data Assimilation

- We do not want to rely only on the model forecasts to track the large-scale vortices (i.e. estimate the "true" vortex trajectories)
- Suppose that we observe only (noisy) trajectories of passive tracers (or drifters/floats)
- Deployment strategy: Where should we initialize the tracers?
- Can we use some dynamical structures (e.g. LCS or finite-time coherent sets) to aid the design of the launching strategy?
- Do (optimal) launching strategies depend on assimilation methods?

Recursive Estimation

- Given the data $y_{1:t} := (y_1, \ldots, y_t)$, inference about x_t is carried out by

$$P(x_t|y_{1:t}) \propto P(y_t|x_t, y_{1:t-1})P(x_t|y_{1:t-1})$$

- The normalization term is omitted here
- Prior distribution: (deterministic/stochastic) model containing uncertainties in model itself or initial conditions or both
- Likelihood: uncertainties in predicting y_t from x_t (e.g. $y_t = Hx_t +$"noise")
- Posterior distribution: "combined knowledge", saying nothing about "truth"

Kalman Filtering

- Optimal for"linear + Gaussian" assumption
- KF: "linearly regresses" observation increments onto state variable increments

$$
\begin{aligned}
x^a(t_k) &= x^f(t_k) + \mathbf{K}(t_k)(y^o(t_k) - y^f(t_k)) \\
\mathbf{P}^a(t_k) &= (\mathbf{I} - \mathbf{K}(t_k)\mathbf{H})\mathbf{P}^f(t_k) \\
y^f(t_k) &= \mathbf{H}x^f(t_k) + \epsilon(t_k) \\
\mathbf{K}(t_k) &= \mathbf{P}^f(t_k)\mathbf{H}^T(\mathbf{H}\mathbf{P}^f(t_k)\mathbf{H}^T + \mathbf{R})^{-1}
\end{aligned}
$$

- $x^f(t_k)$ and $\mathbf{P}^f(t_k)$ come from the model forecast
- $\epsilon(t_k)$ is observation noise with known covariance $\mathbf{R}$
- Provide only mean x^a and covariance matrix $\mathbf{P}^a$ (so-called the "uncertainty")

Ensemble KF (ENKF) with perturbed obsevation

- ENKF: use sample statistics to approximate $\mathbf{P}^a$ and $\mathbf{P}^f$
- Anomalies: $\mathbf{X} = [x_1|\ldots|x_N]/\sqrt{N-1}$

$$x_i^a(t_k) = x_i^f(t_k) + \mathbf{K}_e(t_k)(\underbrace{y^o(t_k) + \epsilon_i(t_k)}_{y_i} - \underbrace{\mathbf{H}x_i^f(t_k)}_{y_i^f(t_k)})$$

$$\mathbf{P}_e^f(t_k) = \mathbf{X}\mathbf{X}^T, \quad \mathbf{P}_e^a(t_k) \to (\mathbf{I} - \mathbf{K}_e(t_k)\mathbf{H})\mathbf{P}_e^f(t_k)$$

$$\mathbf{K}_e(t_k) = \mathbf{X}^f(\mathbf{Y}^f)^T(\mathbf{Y}^t(\mathbf{Y}^f)^T + \mathbf{Y}\mathbf{Y}^T)^{-1}$$

- $\mathbf{P}_e^a(t_k)$ converges to the desired form when N large and x^f and ϵ_i uncorrelated
- Use the ensemble mean $\langle x_i^a \rangle$ as the state estimate

Important Sampling (IS)

- Suppose we can draw $x^{(i)} \overset{i.i.d.}{\sim} \pi(x)$,

$$\mathbb{E}_\pi[f] = \int f(x)\pi(x)dx \approx N^{-1}\sum_{i=1}^{N} f(x^{(i)})\delta(x - x^{(i)})$$

- we have an empirical distribution

$$\widehat{\pi} = N^{-1}\sum_{i=1}^{N} \delta(x - x^{(i)})$$

- IS: Suppose $x^{(i)} \overset{i.i.d.}{\sim} \pi(x)$ is unavailable and $\pi(x)$ can be evaluated only up to a normalization constant so that $\pi(x) = \tilde{\pi}(x)/Z_p$
- Choose "proposal density" $q(x) = \tilde{q}(x)/Z_q$ such that $\pi(x) > 0 \Rightarrow q(x) > 0$

Important Sampling (IS)

- Draw $x^{(i)} \overset{i.i.d.}{\sim} \tilde{q}(x)$

$$E_\pi[f] = \int f(x)\frac{\pi(x)}{\tilde{q}(x)}\tilde{q}(x)dx \approx \frac{Z_q}{Z_p}\sum_{i=1}^{N} f(x^{(i)})\tilde{w}^{(i)}; \quad \tilde{w}^{(i)} = \frac{\tilde{\pi}(x)}{\tilde{q}(x)}$$

- The normalization can be evaluated with the same $x^{(i)}$

$$\frac{Z_p}{Z_q} = \frac{1}{Z_q}\int \frac{\tilde{\pi}(x)}{d}x = \int \frac{\tilde{\pi}(x)}{\tilde{q}(x)}\frac{\tilde{q}(x)}{Z_q}dx \approx \sum_{i=1}^{N}\tilde{w}^{(i)}$$

- The empirical distribution is now a weighted sum

$$\widehat{\pi} = \sum_{i=1}^{N} w^{(i)}\delta(x - x^{(i)}); \qquad w^{(i)} = \frac{\tilde{w}^{(i)}}{\sum_{i=1}^{N}\tilde{w}^{(i)}},$$

- $w^{(i)}$ compensate the discrepancy between $q(x)$ and $\pi(x)$

Sequential Important Sampling (SIS)

- $P(x_{0:t}, y_{1:t}) = P(x_0)P(x_1|x_0)P(y_1|x_1)\cdots P(x_t|x_{t-1})P(y_t|x_t)$
- Our target: $P(x_{0:t}|y_{1:t})$ (can be marginalized to $P(x_t|y_{1:t})$)
- Choose $q(x_{0:t}|y_{1:t})$ such that $x_{0:t}^{(i)}$ can be drawn without modifying the past trajectories $x_{0:t-1}^{(i)}$

$$
\begin{aligned}
q(x_{0:t}|y_{1:t}) &= q(x_{0:t-1}|y_{1:t-1})q(x_t|x_{0:t-1}, y_{1:t}) \\
&= q(x_0)\prod_{k=1}^{t} q(x_k|x_{0:k-1}, y_{1:k})
\end{aligned}
$$

- If $x_{0:t-1}^{(i)} \sim q(x_{0:t-1}|y_{1:t-1})$ and $x_t^{(i)} \sim q(x_t|x_{0:t-1}^{(i)}, y_{1:t})$, then $x_{0:t}^{(i)} \equiv (x_t^{(i)}, x_{0:t-1}^{(i)}) \sim q(x_{0:t}|y_{1:t})$.

Sequential Important Sampling (SIS)

- Choose $x_0^{(i)} \sim q_0(x_0) = P(x_0)$ and $x_1^{(i)} \sim q(x_1|x_0^{(i)}, y_1)$,

$$w_1^{(i)} = \frac{P(x_{0:1}^{(i)}|y_1)}{q(x_{0:1}^{(i)}|y_1)} \propto \frac{\cancel{P(x_0^{(i)})}P(x_1^{(i)}|x_0^{(i)})P(y_1|x_1^{(i)})}{\cancel{q_0(x_0^{(i)})}q(x_1^{(i)}|x_0^{(i)}, y_1)}$$

$$w_2^{(i)} = \frac{P(x_{0:2}^{(i)}|y_{1:2})}{q(x_{0:2}^{(i)}|y_{1:2})} \propto \frac{P(x_{0:1}^{(i)}|y_1)P(x_2^{(i)}|x_1^{(i)})P(y_2|x_2^{(i)})}{q(x_{0:1}^{(i)}|y_1)q(x_t^{(i)}|x_{0:1}^{(i)}, y_{1:2})}$$

$$= w_1^{(i)} \frac{P(x_2^{(i)}|x_1^{(i)})P(y_2|x_2^{(i)})}{q(x_2^{(i)}|x_{0:1}^{(i)}, y_{1:2})}; \qquad x_2^{(i)} \sim q(x_2|x_{0:1}^{(i)}, y_{1:2})$$

- At time t:

$$w_t^{(i)} = w_{t-1}^{(i)} \frac{P(x_t^{(i)}|x_{t-1}^{(i)})P(y_t|x_t^{(i)})}{q(x_t^{(i)}|x_{0:t-1}^{(i)}, y_{1:t})}; \qquad x_t^{(i)} \sim q(x_t|x_{0:t-1}^{(i)}, y_{1:t})$$

“Standard” Particle filtering

- Choose $q(x_t^{(i)}|x_{0:t-1}^{(i)}, y_t) = p(x_t^{(i)}|x_{t-1}^{(i)})$. We get

$$w_t^{(i)} \propto w_{t-1}^{(i)} p(y_t|x_t^{(i)})$$

- This is an easy choice, but not the “optimal" choice.
- Then, the posterior density at n is

$$p(x_{0:t}|y_{1:t}) \approx \sum_{i=1}^{N} w_t^{(i)} \delta(x_{0:t} - x_{0:t}^{(i)})$$

- It is easy to marginalize

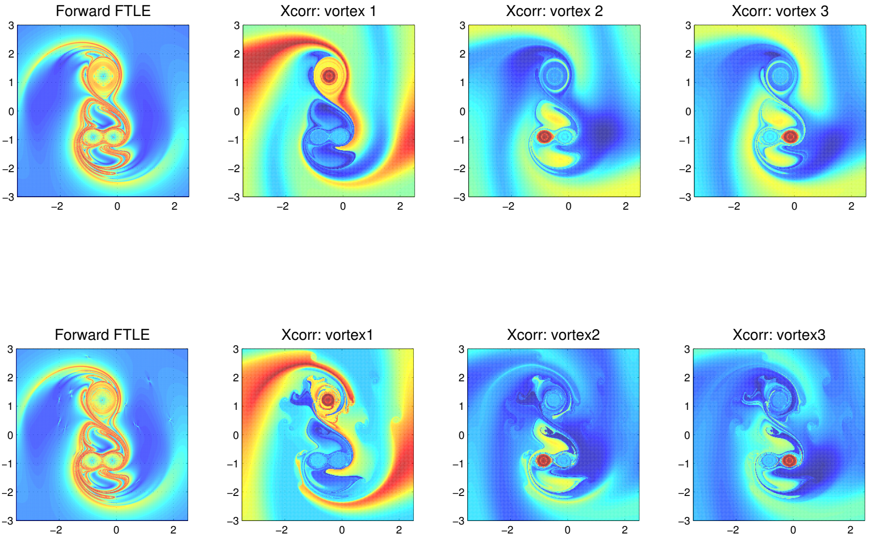
$$p(x_t|y_{1:t}) \approx \sum_{i=1}^{N} w_t^{(i)} \delta(x_t - x_t^{(i)})$$

- In practice, resampling is required

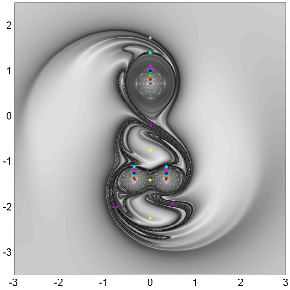
Truth and Model Forecast

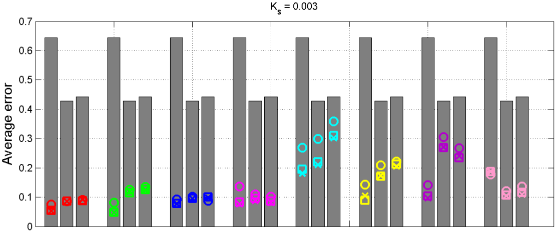
- Vortices: $[x_1, y_1, \ldots, x_m, y_m] \equiv \mathbf{x}_F$
- Tracers: $[z_{x,1}, z_{y,1}, \ldots, z_{x,n}, z_{y,n}] \equiv \mathbf{x}_D$
- State variable: $(\mathbf{x}_F, \mathbf{x}_D)$
- Model uncertainty: SDE with $N(0, 0.05\mathbf{I})$ for a model forecast
- Observation: $(\mathbf{x}_D)+$"noise"
- Observation noise: Gaussian with zero mean and covariance $0.05\mathbf{I}$

Truth and Model Forecast



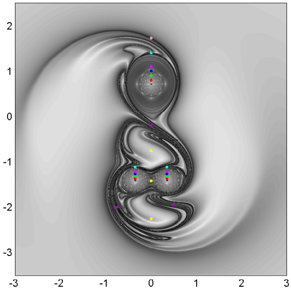
Results: ENKF

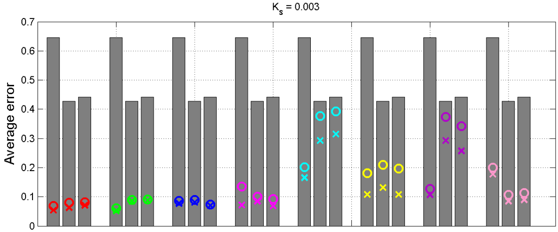




Circle: ENKF 30 pts, Square: ENKF 300 pts, Cross: ENKF 1000pts

Results: PF





Circle: PF 400 pts, Cross: PF 2000pts