SDE4DVar

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1 Formulation

SDE and observation model

$$x^{(1)} \sim N(0, E_1) \tag{1}$$

$$x^{(t)} = M(x^{(t-1)}, p) + \xi^{(t)}, \xi^{(t)} \sim N(0, E), t = 2, \cdots, T$$
(2)

$$y^{(t)} = H(x^{(t)}, r) + \xi'^{(t)}, \xi'^{(t)} \sim N(0, \Sigma), t = 1, \cdots, T$$
(3)

Maximul path

$$\operatorname{Max}_{x^{(1:T)}} p(x^{(1:T)}, y^{(1:T)} | \mu) = p(x^{(1)} | \mu) p(y^{(1)} | x^{(1)}) \prod_{t=2}^{T} p(x^{(t)} | x^{(t-1)}) p(y^{(t)} | x^{(t)})$$
(4)

$$\operatorname{Min}_{x^{(1:T)}} l(x^{(1:T)}, y^{(1:T)} | \mu)$$
 (5)

$$= -\ln p(x^{(1:T)}, y^{(1:T)}|\mu) \tag{6}$$

$$= \frac{1}{2} \ln |E_1| + \frac{T-1}{2} \ln |E| + \frac{T}{2} \ln |\Sigma| + \frac{1}{2} (x^{(1)} - \mu)^{\mathrm{T}} E_1^{-1} (x^{(1)} - \mu)$$

$$+ \frac{1}{2} \sum_{t=2}^{I} (x^{(t)} - M(x^{(t-1)}, p))^{\mathrm{T}} E^{-1} (x^{(t)} - M(x^{(t-1)}, p))$$

$$+\frac{1}{2}\sum_{t=1}^{T}(H(x^{(t)},r)-y^{(t)})^{\mathrm{T}}\Sigma^{-1}(H(x^{(t)},r)-y^{(t)})$$
(7)

$$\frac{\partial l}{\partial x^{(1)}} = E_1^{-1}(x^{(1)} - \mu) + \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \Sigma^{-1}(H(x^{(1)}, r) - y^{(1)}) = 0
+ \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1}(M(x^{(1)}, p) - x^{(2)}) = 0$$
(8)

$$\frac{\partial l}{\partial x^{(t)}} = E^{-1}(x^{(t)} - M(x^{(t-1)}, p)) + \left(\frac{\partial H}{\partial x^{(t)}}\right)^{\mathrm{T}} \Sigma^{-1}(H(x^{(t)}, r) - y^{(t)})
+ \left(\frac{\partial M}{\partial x^{(t)}}\right)^{\mathrm{T}} E^{-1}(M(x^{(t)}, p) - x^{(t+1)}) = 0 \ (t = 2, \dots, T - 1) \tag{9}$$

Cost function

$$J(x^{(1)}, p, r) = \mathcal{J}(x^{(1:T)}, p, r) = l(x^{(1:T)}, y^{(1:T)} | \mu) + \text{Regularization}$$
(10)

$$\begin{aligned} & \text{Min}_{x^{(1:T)}, p, r} L(x^{(1:T)}, p, r; \lambda^{(2:T)}) = \mathcal{J}(x^{(1:T)}, p, r) \\ & + \lambda^{(2)T} \Big(E_1^{-1}(x^{(1)} - \mu) + \left(\frac{\partial H}{\partial x^{(1)}} \right)^T \Sigma^{-1} (H(x^{(1)}, r) - y^{(1)}) \\ & + \left(\frac{\partial M}{\partial x^{(1)}} \right)^T E^{-1} (M(x^{(1)}, p) - x^{(2)}) \Big) \\ & + \sum_{t=2}^{T-1} \lambda^{(t+1)T} \Big(E^{-1}(x^{(t)} - M(x^{(t-1)}, p)) + \left(\frac{\partial H}{\partial x^{(1)}} \right)^T \Sigma^{-1} (H(x^{(1)}, r) - y^{(1)}) \\ & + \left(\frac{\partial M}{\partial x^{(t)}} \right)^T E^{-1} (M(x^{(t)}, p) - x^{(t+1)}) \Big) \end{aligned}$$
(11)

Orbit calculation

$$x^{(2)} - M(x^{(1)}, p) = \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1} \setminus \left\{ E_{1}^{-1}(x^{(1)} - \mu) + \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \Sigma^{-1}(H(x^{(1)}, r) - y^{(1)}) \right\}$$

$$(12)$$

$$x^{(t+1)} - M(x^{(t)}, p) = \left(\frac{\partial M}{\partial x^{(t)}}\right)^{\mathrm{T}} E^{-1} \setminus \left\{ E^{-1}(x^{(t)} - M(x^{(t-1)}, p)) + \left(\frac{\partial H}{\partial x^{(t)}}\right)^{\mathrm{T}} \Sigma^{-1}(H(x^{(t)}, r) - y^{(t)}) \right\}$$

$$(t = 2, \dots, T - 1)$$

$$(13)$$

Gradient calculation

$$\lambda^{(T+1)} = 0 \qquad (14)$$

$$\lambda^{(T)} = E^{-1} \frac{\partial M}{\partial x^{(T-1)}} \backslash \frac{\partial \mathcal{J}(x^{(1:T)}, p, r)}{\partial x^{(T)}} \qquad (15)$$

$$\lambda^{(t)} = E^{-1} \frac{\partial M}{\partial x^{(t-1)}} \backslash \left[\left\{ E^{-1} + \left(\frac{\partial H}{\partial x^{(t)}} \right)^{\mathrm{T}} \Sigma^{-1} \frac{\partial H}{\partial x^{(t)}} + \left(\frac{\partial M}{\partial x^{(t)}} \right)^{\mathrm{T}} E^{-1} \frac{\partial M}{\partial x^{(t)}} \right\} \lambda^{(t+1)} - \left(\frac{\partial M}{\partial x^{(t)}} \right)^{\mathrm{T}} E^{-1} \lambda^{(t+2)}$$

$$+ \left(\frac{\partial^{2} H}{\partial x^{(t)^{2}}} \lambda^{(t+1)} \right)^{\mathrm{T}} \Sigma^{-1} (H(x^{(t)}, r) - y^{(t)}) - \left(\frac{\partial^{2} M}{\partial x^{(t)^{2}}} \lambda^{(t+1)} \right)^{\mathrm{T}} E^{-1} (x^{(t+1)} - M(x^{(t)})) \right] (t = T - 1, \cdots, 2)$$

$$(16)$$

$$\frac{\partial J(x^{(1)}, p, r)}{\partial x^{(1)}} = \left\{ E_{1}^{-1} + \left(\frac{\partial H}{\partial x^{(1)}} \right)^{\mathrm{T}} \Sigma^{-1} \frac{\partial H}{\partial x^{(1)}} + \left(\frac{\partial M}{\partial x^{(1)}} \right)^{\mathrm{T}} E^{-1} \frac{\partial M}{\partial x^{(1)}} \right\} \lambda^{(2)} - \left(\frac{\partial M}{\partial x^{(1)}} \right)^{\mathrm{T}} E^{-1} \lambda^{(3)}$$

$$+ \left(\frac{\partial^{2} H}{\partial x^{(1)^{2}}} \lambda^{(2)} \right)^{\mathrm{T}} \Sigma^{-1} (H(x^{(1)}, r) - y^{(1)}) - \left(\frac{\partial^{2} M}{\partial x^{(1)^{2}}} \lambda^{(2)} \right)^{\mathrm{T}} E^{-1} (x^{(2)} - M(x^{(1)}))$$

$$(17)$$

$$\frac{\partial J(x^{(1)}, p, r)}{\partial p} = \sum_{t=1}^{T-1} \left\{ \left(\frac{\partial M^{(t)}}{\partial p} \right)^{\mathrm{T}} E^{-1} \left(\frac{\partial M}{\partial x^{(t)}} \lambda^{(t+1)} - \lambda^{(t+2)} + M(x^{(t)}, p) - x^{(t+1)} \right) - \left(\frac{\partial^{2} M}{\partial p \partial x^{(t)}} \lambda^{(t+1)} \right)^{\mathrm{T}} E^{-1} (x^{(t+1)} - M(x^{(t)}, p)) \right\} + \text{Regularizationg radient}$$

$$\frac{\partial J(x^{(1)}, p, r)}{\partial r} = \sum_{t=1}^{T} \left\{ \left(\frac{\partial^{2} H}{\partial r \partial x^{(t)}} \lambda^{(t+1)} \right)^{\mathrm{T}} \Sigma^{-1} (H(x^{(t)}, r) - y^{(t)}) + \text{Regularizationg radient} \right\}$$

$$+ \left(\frac{\partial H^{(t)}}{\partial r} \right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial H}{\partial x^{(t)}} \lambda^{(t+1)} + H(x^{(t)}, r) - y^{(t)} \right) + \text{Regularization gradient}$$

$$(18)$$

where

$$\frac{\partial \mathcal{J}(x^{(1:T)}, p, r)}{\partial x^{(T)}} = E^{-1}(x^{(T)} - M(x^{(T-1)}, p)) + \left(\frac{\partial H}{\partial x^{(T)}}\right)^{\mathrm{T}} \Sigma^{-1}(H(x^{(T)}, r) - y^{(T)})$$
(20)

Neighboring orbit calculation

$$\delta x^{(2)} - \frac{\partial M}{\partial x^{(1)}} \delta x^{(1)} - \frac{\partial M^{(1)}}{\partial p} \delta p$$

$$= \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1} \setminus \left\{ -\left(\frac{\partial^{2} M}{\partial x^{(1)2}} \delta x^{(1)} + \frac{\partial^{2} M}{\partial x^{(1)} \partial p} \delta p\right)^{\mathrm{T}} E^{-1} (x^{(2)} - M(x^{(1)}, p)) + E_{1}^{-1} \delta x^{(1)} + \left(\frac{\partial^{2} H}{\partial x^{(1)2}} \delta x^{(1)} + \frac{\partial^{2} H}{\partial x^{(1)} \partial r} \delta r\right)^{\mathrm{T}} \Sigma^{-1} (H(x^{(1)}, r) - y^{(1)}) + \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial H}{\partial x^{(1)}} \delta x^{(1)} + \frac{\partial H^{(1)}}{\partial r} \delta r\right) \right\}$$

$$\delta x^{(t+1)} - \frac{\partial M}{\partial x^{(t)}} \delta x^{(t)} - \frac{\partial M^{(t)}}{\partial p} \delta p$$

$$= \left(\frac{\partial M}{\partial x^{(t)}}\right)^{\mathrm{T}} E^{-1} \setminus \left\{ -\left(\frac{\partial^{2} M}{\partial x^{(t)2}} \delta x^{(t)} + \frac{\partial^{2} M}{\partial x^{(t)} \partial p} \delta p\right)^{\mathrm{T}} E^{-1} (x^{(t+1)} - M(x^{(t)}, p)) + E^{-1} \left(\delta x^{(t)} - \frac{\partial M}{\partial x^{(t-1)}} \delta x^{(t-1)} - \frac{\partial M^{(t-1)}}{\partial p} \delta p\right) + \left(\frac{\partial^{2} H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^{2} H}{\partial x^{(t)} \partial r} \delta r\right)^{\mathrm{T}} \Sigma^{-1} (H(x^{(t)}, r) - y^{(t)}) + \left(\frac{\partial H}{\partial x^{(t)}}\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial H^{(t)}}{\partial r} \delta r\right) \right\}$$

$$(t = 2, \dots, T - 1) \tag{22}$$

Hessian-vector product calculation

$$\delta\lambda^{(T+1)} = 0 \tag{23}$$

$$\delta\lambda^{(T)} = E^{-1} \frac{\partial M}{\partial x^{(T-1)}} \setminus \left\{ -E^{-1} \left(\frac{\partial^2 M}{\partial x^{(T-1)}} \delta x^{(T-1)} + \frac{\partial^2 M}{\partial x^{(T-1)} \partial p} \delta p \right) \lambda^{(T)} + E^{-1} \left(\delta x^{(T)} - \frac{\partial M}{\partial x^{(T-1)}} \delta x^{(T-1)} - \frac{\partial M^{(T-1)}}{\partial p} \delta p \right) \lambda^{(T)} + E^{-1} \left(\delta x^{(T)} - \frac{\partial M}{\partial x^{(T-1)}} \delta x^{(T-1)} - \frac{\partial M^{(T-1)}}{\partial p} \delta p \right) + \left(\frac{\partial^2 H}{\partial x^{(T)}} \delta x^{(T)} + \frac{\partial^2 H}{\partial x^{(T)} \partial r} \delta r \right)^T \sum^{-1} \left(H(x^{(T)}, r) - y^{(T)} \right) + \left(\frac{\partial H}{\partial x^{(T)}} \right)^T \sum^{-1} \left(\frac{\partial H}{\partial x^{(T)}} \delta x^{(T)} + \frac{\partial H^{(T)}}{\partial r} \delta r \right) \right\} \tag{24}$$

$$\delta\lambda^{(t)} = E^{-1} \frac{\partial M}{\partial x^{(t-1)}} \setminus \left[-E^{-1} \left(\frac{\partial^2 M}{\partial x^{(t-1)}} \delta x^{(t-1)} + \frac{\partial^2 M}{\partial x^{(t-1)}} \delta p \right) \lambda^{(t)} + \left(\frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H^{(t)}}{\partial x^{(t)}} \delta r \right)^T \sum^{-1} \frac{\partial H}{\partial x^{(t)}} + \left(\frac{\partial H}{\partial x^{(t)}} \right)^T \sum^{-1} \left(\frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H^{(t)}}{\partial x^{(t)}} \delta r \right) + \left(\frac{\partial^2 M}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 M}{\partial x^{(t)}} \delta p \right)^T E^{-1} \frac{\partial M}{\partial x^{(t)}} + \left(\frac{\partial H}{\partial x^{(t)}} \right)^T \sum^{-1} \left(\frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 M^{(t)}}{\partial x^{(t)}} \delta p \right) \right\} \lambda^{(t+1)} + \left\{ E^{-1} + \left(\frac{\partial H}{\partial x^{(t)}} \right)^T \sum^{-1} \frac{\partial H}{\partial x^{(t)}} + \left(\frac{\partial M}{\partial x^{(t)}} \right)^T E^{-1} \delta \lambda^{(t+1)} - \left(\frac{\partial^2 M}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t+1)} \right\}^T \sum^{-1} \delta \lambda^{(t+2)} + \left\{ \left(\frac{\partial^3 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^3 H}{\partial x^{(t)}} \delta p \right) \lambda^{(t+1)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} - \frac{\partial H^{(t)}}{\partial r} \delta r \right\} \lambda^{(t+1)} \right\}^T \sum^{-1} \left(\frac{\partial^3 H}{\partial x^{(t)}} \delta x^{(t+1)} - \frac{\partial^3 H}{\partial x^{(t)}} \delta p \right) \lambda^{(t+1)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} - \frac{\partial M^{(t)}}{\partial r} \delta p \right) \right\} \lambda^{(t+1)}$$

$$- \left(\frac{\partial^3 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial^3 H}{\partial x^{(t)}} \delta p \right) \lambda^{(t+1)} + \frac{\partial^2 H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial H^{(t)}}{\partial r} \delta r \right) \lambda^{(t+1)} - \left(\frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} - \frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} \right) \lambda^{(t+1)} + \left(\frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} \right) \lambda^{(t+1)} +$$

$$\begin{split} \delta\left(\frac{\partial J(x^{(1)},p,r)}{\partial x^{(1)}}\right) &= \left\{\left(\frac{\partial^2 H}{\partial x^{(1)^2}}\delta x^{(1)} + \frac{\partial^2 H^{(1)}}{\partial x^{(1)}}\delta r\right)^{\mathrm{T}} \sum^{-1} \frac{\partial H}{\partial x^{(1)}} \\ &+ \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \sum^{-1} \left(\frac{\partial^2 H}{\partial x^{(1)^2}}\delta x^{(1)} + \frac{\partial^2 H^{(1)}}{\partial x^{(1)}\partial r}\delta r\right) \\ &+ \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \sum^{-1} \left(\frac{\partial^2 H}{\partial x^{(1)^2}}\delta x^{(1)} + \frac{\partial^2 H^{(1)}}{\partial x^{(1)}\partial p}\delta p\right)^{\mathrm{T}} E^{-1} \frac{\partial M}{\partial x^{(1)}} \\ &+ \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1} \left(\frac{\partial^2 M}{\partial x^{(1)^2}}\delta x^{(1)} + \frac{\partial^2 M^{(1)}}{\partial x^{(1)}\partial p}\delta p\right)^{\mathrm{T}} E^{-1} \frac{\partial M}{\partial x^{(1)}} \\ &+ \left\{E^{-1} + \left(\frac{\partial H}{\partial x^{(1)}}\right)^{\mathrm{T}} \sum^{-1} \frac{\partial H}{\partial x^{(1)}} + \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1} \frac{\partial M}{\partial x^{(1)}} \right\} \delta \lambda^{(2)} \\ &- \left(\frac{\partial^2 M}{\partial x^{(1)^2}}\delta x^{(1)} + \frac{\partial^2 M^{(1)}}{\partial x^{(1)}\partial p}\delta p\right)^{\mathrm{T}} E^{-1} \lambda^{(3)} - \left(\frac{\partial M}{\partial x^{(1)}}\right)^{\mathrm{T}} E^{-1} \delta \lambda^{(3)} \\ &+ \left\{\left(\frac{\partial^3 H}{\partial x^{(1)^3}}\delta x^{(1)} + \frac{\partial^3 H}{\partial x^{(1)^2}\partial p}\delta r\right) \lambda^{(2)} + \frac{\partial^2 H}{\partial x^{(1)^2}}\delta \lambda^{(2)}\right\}^{\mathrm{T}} \sum^{-1} (H(x^{(1)},r) - y^{(1)}) \\ &+ \left(\frac{\partial^2 H}{\partial x^{(1)^3}}\delta x^{(1)} + \frac{\partial^3 M}{\partial x^{(1)^2}\partial p}\delta p\right) \lambda^{(2)} + \frac{\partial^2 M}{\partial x^{(1)^2}}\delta \lambda^{(2)}\right\}^{\mathrm{T}} E^{-1} (x^{(2)} - M(x^{(1)},p)) \\ &- \left(\frac{\partial^2 M}{\partial x^{(1)}}\lambda^{(2)}\right)^{\mathrm{T}} E^{-1} \left(\delta x^{(2)} - \frac{\partial M}{\partial x^{(1)}}\delta x^{(1)} - \frac{\partial M^{(1)}}{\partial p}\delta p\right) \qquad (26) \\ &\delta \left(\frac{\partial J(x^{(1)},p,r)}{\partial p}\right) \\ &= \sum_{t=1}^{T-1} \left[\left(\frac{\partial^2 M}{\partial p\partial x^{(t)}}\delta x^{(t)} + \frac{\partial^2 M^{(t)}}{\partial p^2}\delta p\right)^{\mathrm{T}} E^{-1} \left(\frac{\partial M}{\partial x^{(1)}}\lambda^{(t+1)} - \lambda^{(t+2)} + M(x^{(t)},p) - x^{(t+1)}\right) \\ &+ \left(\frac{\partial M}{\partial p}(\delta) \lambda^{(t+1)} + \delta x^{(t)}\right) + \frac{\partial M^{(t)}}{\partial p}\delta p - \delta \lambda^{(t+1)} - \delta x^{(t+1)}\right\}^{\mathrm{T}} E^{-1} \left(\lambda^{(t+1)} - M(x^{(t)},p)\right) \\ &- \left(\left(\frac{\partial^3 M}{\partial p\partial x^{(t)}}\lambda^{(t+1)} + \frac{\partial^3 M}{\partial p\partial x^{(t)}\partial p}\delta p\right) \lambda^{(t+1)} + \frac{\partial^2 M}{\partial p}\delta x^{(t)} \delta x^{(t)} + \frac{\partial^2 M}{\partial p\partial x^{(t)}}\delta x^{(t)} + \frac{\partial^2 M}{\partial p\partial x^{(t)}}\delta x^{(t)} - \frac{\partial M}{\partial p}\delta x^{(t)}\right) + \delta \mathrm{Regularizationg radient} \end{split}$$

$$\begin{split} \delta\left(\frac{\partial J(x^{(1)},p,r)}{\partial r}\right) \\ &= \sum_{t=1}^{T-1} \Big[\left(\frac{\partial^2 H}{\partial r \partial x^{(t)}} \delta x^{(t)} + \frac{\partial^2 H^{(t)}}{\partial r^2} \delta r\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial H}{\partial x^{(t)}} \lambda^{(t+1)} + H(x^{(t)},r) - y^{(t)}\right) \\ &\quad + \left(\frac{\partial H^{(t)}}{\partial r}\right)^{\mathrm{T}} \Sigma^{-1} \Big\{ \left(\frac{\partial^2 H}{\partial x^{(t)2}} \delta x^{(t)} + \frac{\partial^2 H^{(t)}}{\partial x^{(t)} \partial r} \delta r\right) \lambda^{(t+1)} \\ &\quad + \frac{\partial H}{\partial x^{(t)}} \left(\delta \lambda^{(t+1)} + \delta x^{(t)}\right) + \frac{\partial H^{(t)}}{\partial r} \delta r \Big\} \\ &\quad + \Big\{ \left(\frac{\partial^3 H}{\partial r \partial x^{(t)2}} \delta x^{(t)} + \frac{\partial^3 H}{\partial r \partial x^{(t)} \partial r} \delta r\right) \lambda^{(t+1)} + \frac{\partial^2 H}{\partial r \partial x^{(t)}} \delta \lambda^{(t+1)} \Big\}^{\mathrm{T}} \Sigma^{-1} (H(x^{(t)},r) - y^{(t)}) \\ &\quad + \left(\frac{\partial^2 H}{\partial r \partial x^{(t)}} \lambda^{(t+1)}\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial H}{\partial x^{(t)}} \delta x^{(t)} + \frac{\partial H^{(t)}}{\partial r} \delta r\right) \Big] + \delta \mathrm{Regularization gradient} \end{split} \tag{28}$$