“Ensemblized” linear least squares (LLS)

Patrick N. Raanes

ISDA-Online
Jan. 20, 2023


LLS
LIGHTYEAR
EVERYWHERE

Iter. ens uses LLS

Iter. ens uses LLS

EnKF uses LLS

Iter. ens uses LLS
EnKF uses LLS
EAKF, ETKF uses LLS

Iter. ens
uses LLS

EnKF
uses LLS

EAKF, ETKF
uses LLS

EnKF
is LLS

Iter. ens uses LLS

EnKF uses LLS

EAKF, ETKF uses LLS

EnKF is LLS

LLS $\Rightarrow$ avrg. grad

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,
$$\bar{\mathbf{C}}_{y,x} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$
$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as
$$\bar{\nabla} f := \bar{\mathbf{C}}_{y,x}\, \bar{\mathbf{C}}_{x}^{+} \tag{3}$$
$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} (\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$
$$(\qquad)$$

- ML
- If $N \le d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,
$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$
$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$
$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} (\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}}(\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

( )

- ML
- If $N \le d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}}(\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

- ML
- If $N \le d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} (\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\mathsf{T} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^\mathsf{T} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^\mathsf{T}(\mathbf{X}\,\mathbf{X}^\mathsf{T})^{+} \tag{4}$$

$$(\mathbf{A}^{+} = \mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^\mathsf{T} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\mathsf{T} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^\mathsf{T} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^\mathsf{T} (\mathbf{X}\,\mathbf{X}^\mathsf{T})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^\mathsf{T} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\mathsf{T} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^\mathsf{T} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^\mathsf{T}(\mathbf{X}\,\mathbf{X}^\mathsf{T})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+} \,. \qquad (\mathbf{A}^{+} = \mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^\mathsf{T} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} \coloneqq \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f \coloneqq \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\,\bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}}(\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+})$$

- ML
- If $N \le d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}}\,[\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}}(\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}}\,[\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^{\mathsf{T}} (\mathbf{X}\,\mathbf{X}^{\mathsf{T}})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^{\mathsf{T}} [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,

$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\mathsf{T} \tag{1}$$

$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^\mathsf{T} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$

$$= \mathbf{Y}\,\mathbf{X}^\mathsf{T}(\mathbf{X}\,\mathbf{X}^\mathsf{T})^{+} \tag{4}$$

$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^\mathsf{T}\, [\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Covariances and LLS regression

Let $f(\boldsymbol{x}) = \boldsymbol{y}$.

Let $\mathbf{X}$ and $\mathbf{Y}$ be *centred* ensemble matrices: n-th column is $\boldsymbol{x}_n - \bar{\boldsymbol{x}}$ and $\boldsymbol{y}_n - \bar{\boldsymbol{y}}$.

Recall covariance estimate,
$$\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} := \frac{1}{N-1} \sum_n (\boldsymbol{y}_n - \bar{\boldsymbol{y}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\mathsf{T} \tag{1}$$
$$= \frac{1}{N-1} \mathbf{Y}\,\mathbf{X}^\mathsf{T} \tag{2}$$

Define the ensemble LLS operator $\bar{\nabla}$ as

$$\bar{\nabla} f := \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \tag{3}$$
$$= \mathbf{Y}\,\mathbf{X}^\mathsf{T}(\mathbf{X}\,\mathbf{X}^\mathsf{T})^{+} \tag{4}$$
$$= \mathbf{Y}\mathbf{X}^{+}\,. \qquad (\mathbf{A}^{+} = \mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+})$$

- ML
- If $N \leq d_x$, reproduces increments: $[\boldsymbol{y}_n - \bar{\boldsymbol{y}}] = (\bar{\nabla} f)^\mathsf{T}\,[\boldsymbol{x}_n - \bar{\boldsymbol{x}}]$.
- min-norm LLS, BLUE, MVUE
- Relates to: finite differences (FD), simplex derivatives

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1}(\boldsymbol{\mu} - \boldsymbol{x})$,

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x}-\boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^\top d\boldsymbol{x} + \big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})$,

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^\top d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} + \Big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n} \Big]_{\partial \mathbb{R}^d} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial \mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$
$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})$,

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\ \ \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N \to \infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x}),$$

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x}) \,,$$

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1} \,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= - \int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \xcancel{\left[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\right]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})$,

and so

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^\mathsf{T}\, d\boldsymbol{x} \;+\; \cancel{\big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})\,,$$

and so

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^\mathsf{T}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}\,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \cancel{\big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})\,,$$

and so

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}\,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= - \int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \cancel{\big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})\,,$$

and so

$$\mathbb{E}\, \nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x} \;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}\,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \cancel{\big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But
$$\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$$
$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1}(\boldsymbol{\mu} - \boldsymbol{x})\,,$$

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x} \;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}\,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's lemma

Let $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C}_{\boldsymbol{x}})$, i.e. $p(\boldsymbol{x}) \propto e^{-\|\boldsymbol{x}-\boldsymbol{\mu}\|^2_{\mathbf{C}_{\boldsymbol{x}}}/2}$.

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) := \int_{\mathbb{R}^d} \nabla f(\boldsymbol{x})\, p(\boldsymbol{x})\, d\boldsymbol{x} \tag{5}$$

$$= -\int_{\mathbb{R}^d} f(\boldsymbol{x})\, [\nabla p(\boldsymbol{x})]^{\mathsf{T}}\, d\boldsymbol{x} \;+\; \cancel{\big[f(\boldsymbol{x})\, p(\boldsymbol{x})\, \boldsymbol{n}\big]_{\partial\mathbb{R}^d}} \tag{6}$$

using integration by parts, and $p(\boldsymbol{x}) \xrightarrow[\partial\mathbb{R}^d]{} 0$.

But $\nabla p(\boldsymbol{x}) = p(\boldsymbol{x})\, \nabla \log p(\boldsymbol{x})$

$$= p(\boldsymbol{x})\, \mathbf{C}_{\boldsymbol{x}}^{-1} (\boldsymbol{\mu} - \boldsymbol{x})\,,$$

and so

$$\mathbb{E}\,\nabla f(\boldsymbol{x}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, (\boldsymbol{x} - \boldsymbol{\mu})^{\mathsf{T}}\, d\boldsymbol{x}\;\; \mathbf{C}_{\boldsymbol{x}}^{-1} \tag{7}$$

$$= \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}\,. \tag{8}$$

Lastly, by Slutsky, $\bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}}\, \bar{\mathbf{C}}_{\boldsymbol{x}}^{+} \xrightarrow[N\to\infty]{} \mathbf{C}_{\boldsymbol{y},\boldsymbol{x}}\, \mathbf{C}_{\boldsymbol{x}}^{-1}$.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\,\mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{y,x} &\approx \nabla f(\bar{\boldsymbol{x}})\,\bar{\mathbf{C}}_{x}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\mathbf{Y} \approx \nabla f(\bar{\boldsymbol{x}})\,\mathbf{X}\,,$$
$$\text{i.e.} \quad \bar{\mathbf{C}}_{y,x} \approx \nabla f(\bar{\boldsymbol{x}})\,\bar{\mathbf{C}}_{x}\,,$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\mathbf{Y} \quad \approx \nabla f(\bar{\boldsymbol{x}})\,\mathbf{X}\,,$$

$$\text{i.e.} \quad \bar{\mathbf{C}}_{y,x} \approx \nabla f(\bar{\boldsymbol{x}})\,\bar{\mathbf{C}}_{x}\,,$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\,\mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\,\bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\, \nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\, \mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\, \bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\, \nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\, \mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\, \bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\, \mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\, \bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\,\nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N} \tag{9}$$

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\,\mathbf{X}\,, \\ \text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\,\bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019): $\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\, \nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N}$ (9)

Provides link to analytic gradient, ∇f.

Better than solving order-1 Taylor @ mean:

$$\mathbf{Y} \approx \nabla f(\bar{\boldsymbol{x}})\, \mathbf{X}\,,$$

$$\text{i.e.} \quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} \approx \nabla f(\bar{\boldsymbol{x}})\, \bar{\mathbf{C}}_{\boldsymbol{x}}\,,$$

because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Stein's advantages

Raanes et al. (2019):	$\mathbf{Y}\mathbf{X}^{+} =: \bar{\nabla} f \xrightarrow[N\to\infty]{} \mathbb{E}\, \nabla f(\boldsymbol{x}) \quad \text{if } x \sim \mathcal{N}$	(9)
Stordal et al. (2016):	$= \nabla \mathbb{E}\, f(\boldsymbol{x})$	

Provides link to analytic gradient, ∇f.

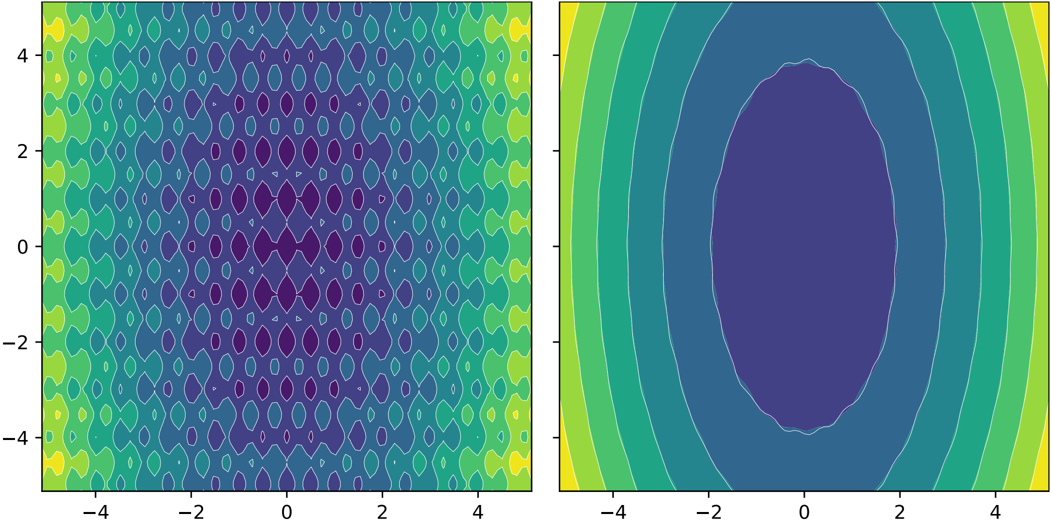
Better than solving order-1 Taylor @ mean:

$$\begin{aligned} \mathbf{Y} &\approx \nabla f(\bar{\boldsymbol{x}})\, \mathbf{X}\,, \\ \text{i.e.}\quad \bar{\mathbf{C}}_{\boldsymbol{y},\boldsymbol{x}} &\approx \nabla f(\bar{\boldsymbol{x}})\, \bar{\mathbf{C}}_{\boldsymbol{x}}\,, \end{aligned}$$

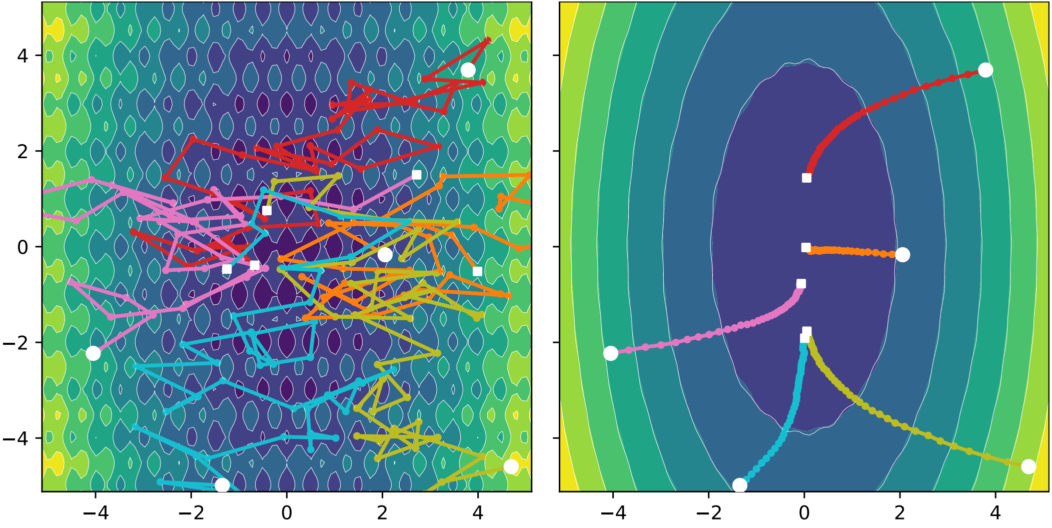
because Stein (9)

- Shows what the *exact* target is.
- Shows that errors *cancel* as $N \to \infty$.
- Enables saying *average sensitivity* without blushing.

Implicit blurring



Implicit blurring




EnKF
Monte-Carlo
+ LLS
imgflip.com

EnKFs use LLS

Recall

EnKFs use LLS

Recall $$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f

EnKFs use LLS

Recall

$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$

$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$

$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{aligned} \bar{\mathbf{C}}_{\boldsymbol{x}} &= \mathbf{X}\mathbf{X}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \bar{\nabla} f &= \mathbf{Y}\mathbf{X}^{+} \end{aligned}$ in $\mathbf{K}$ (10).

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{array}{l} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^{+} \end{array}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

EnKFs use LLS

Recall

$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$

$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}} \, (\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$

$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1} \, . \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^{+} \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases}\mathbf{P} \\ \mathbf{H}\end{cases} \leftarrow \begin{matrix}\bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+\end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases}\mathbf{P} \\ \mathbf{H}\end{cases} \leftarrow \begin{matrix}\bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{I}\end{matrix}$

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} & \leftarrow \quad \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{H} & \leftarrow \quad \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{cases}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} & \leftarrow \quad \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{H} & \leftarrow \quad \mathbf{I} \end{cases}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$,

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$, and apply to obs-update.

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N-1)\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/(N-1) \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/(N-1) \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^{+} \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^{+}$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \mathbf{H} \leftarrow \bar{\nabla} f = \mathbf{Y}\mathbf{X}^{+} \end{cases}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^{\mathsf{T}}/{\scriptstyle (N-1)} \\ \mathbf{H} \leftarrow \mathbf{I} \end{cases}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^{+}$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$ using $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{w}} = \mathbf{I}/{\scriptstyle (N-1)} \\ \mathbf{H} \leftarrow \bar{\nabla}(f \circ \boldsymbol{\phi}) = \mathbf{Y}\,\mathbf{I}^{+} = \mathbf{Y} \end{cases}$

EnKFs use LLS

Recall

$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \quad (10)$$

$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \quad (11)$$

$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N-1)\mathbf{R})^{-1}\,. \quad (12)$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/(N-1) \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/(N-1) \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$ using $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{w}} = \mathbf{I}/(N-1) \\ \bar{\nabla}(f \circ \boldsymbol{\phi}) = \mathbf{Y}\,\mathbf{I}^+ = \mathbf{Y} \end{matrix}$

Then apply $\boldsymbol{\phi}$ to revert to state space.

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^{\mathsf{T}}(\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{T}} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + (N-1)\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^{\mathsf{T}}/(N-1) \\ \mathbf{H} \leftarrow \bar{\nabla} f = \mathbf{Y}\mathbf{X}^{+} \end{cases}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^{\mathsf{T}}/(N-1) \\ \mathbf{H} \leftarrow \mathbf{I} \end{cases}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^{+}$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$ using $\begin{cases} \mathbf{P} \leftarrow \bar{\mathbf{C}}_{\boldsymbol{w}} = \mathbf{I}/(N-1) \\ \mathbf{H} \leftarrow \bar{\nabla}(f \circ \boldsymbol{\phi}) = \mathbf{Y}\,\mathbf{I}^{+} = \mathbf{Y} \end{cases}$

Then apply $\boldsymbol{\phi}$ to revert to state space. Yields $(\bar{\nabla}\boldsymbol{\phi})\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$ using $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{w}} = \mathbf{I}/{\scriptstyle (N-1)} \\ \bar{\nabla}(f \circ \boldsymbol{\phi}) = \mathbf{Y}\,\mathbf{I}^+ = \mathbf{Y} \end{matrix}$

Then apply $\boldsymbol{\phi}$ to revert to state space. Yields $(\bar{\nabla}\boldsymbol{\phi})\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

Could we have anticipated the equivalence?

EnKFs use LLS

Recall
$$\mathbf{K} := \mathbf{P}\mathbf{H}^\mathsf{T}(\mathbf{H}\mathbf{P}\mathbf{H}^\mathsf{T} + \mathbf{R})^{-1} \tag{10}$$
$$\bar{\mathbf{K}} := \bar{\mathbf{C}}_{\boldsymbol{x},\boldsymbol{y}}\,(\bar{\mathbf{C}}_{\boldsymbol{y}} + \mathbf{R})^{-1} \tag{11}$$
$$= \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + {\scriptstyle (N-1)}\mathbf{R})^{-1}\,. \tag{12}$$

As in ***IES***, linearise f, i.e. use $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{x}} = \mathbf{X}\mathbf{X}^\mathsf{T}/{\scriptstyle (N-1)} \\ \bar{\nabla} f = \mathbf{Y}\mathbf{X}^+ \end{matrix}$ in $\mathbf{K}$ (10). Yields $\bar{\mathbf{K}}$ (12). ✓

As in ***EAKF***, first update in obs-space : $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{y}} = \mathbf{Y}\mathbf{Y}^\mathsf{T}/{\scriptstyle (N-1)} \\ \mathbf{I} \end{matrix}$, then compute "reverse" LLS, $\bar{\nabla}^{-1} f := \mathbf{X}\mathbf{Y}^+$, and apply to obs-update. Yields $(\bar{\nabla}^{-1} f)\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

As in ***ETKF***, update in ens. subspace: $\overbrace{\boldsymbol{x} = \bar{\boldsymbol{x}} + \mathbf{X}\boldsymbol{w}}^{\boldsymbol{\phi}(\boldsymbol{w})}$ using $\begin{cases} \mathbf{P} \\ \mathbf{H} \end{cases} \leftarrow \begin{matrix} \bar{\mathbf{C}}_{\boldsymbol{w}} = \mathbf{I}/{\scriptstyle (N-1)} \\ \bar{\nabla}(f \circ \boldsymbol{\phi}) = \mathbf{Y}\,\mathbf{I}^+ = \mathbf{Y} \end{matrix}$
Then apply $\boldsymbol{\phi}$ to revert to state space. Yields $(\bar{\nabla}\boldsymbol{\phi})\,\mathbf{K} = \bar{\mathbf{K}}$. ✓

Could we have anticipated the equivalence?
Yes, by ***chain rule*** (Raanes et al., 2019), i.e. $\bar{\nabla}(f \circ g) = \bar{\nabla} f\ \bar{\nabla} g$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself?

Recall $$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + (N-1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$ yields $$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + \mathbf{D}\mathbf{D}^{\mathsf{T}})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields $$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields $$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{16}$$

$\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+} = \mathbf{A}^{+}$ yields $$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(x) := f(x) + \varepsilon$ yields $$=: \bar{\nabla}^{-1} f_{\text{noisy}}\,. \tag{18}$$

(Snyder, 2015)

$\implies$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\implies$ Can estimate $(x - \bar{x})$ by applying it to $(y - \bar{y})$, i.e.

$$\hat{x}(y) := \bar{x} + \bar{\mathbf{K}}(y - \bar{y}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N-1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx 0$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx 0$ yields $$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+} = \mathbf{A}^{+}$ yields $$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(x) := f(x) + \varepsilon$ yields $$=: \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\implies$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\implies$ Can estimate $(x - \bar{x})$ by applying it to $(y - \bar{y})$, i.e.

$$\hat{x}(y) := \bar{x} + \bar{\mathbf{K}}(y - \bar{y}) \;\checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall
$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + (N-1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall
$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+ \tag{14}$$

$\mathbf{Y}_\text{noisy} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_\text{noisy}\mathbf{Y}_\text{noisy}^\mathsf{T})^+ \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}_\text{noisy}^\mathsf{T}(\mathbf{Y}_\text{noisy}\mathbf{Y}_\text{noisy}^\mathsf{T})^+ \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^+ = \mathbf{A}^+$ yields
$$= \mathbf{X}\mathbf{Y}_\text{noisy}^+ \tag{17}$$

$f_\text{noisy}(x) := f(x) + \varepsilon$ yields
$$=: \bar{\nabla}^{-1} f_\text{noisy} \,. \tag{18}$$

(Snyder, 2015)

$\implies$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_\text{noisy}$ "inverts" model + noise.
$\implies$ Can estimate $(x - \bar{x})$ by applying it to $(y - \bar{y})$, i.e.

$$\hat{x}(y) := \bar{x} + \bar{\mathbf{K}}(y - \bar{y}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall
$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N-1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx 0$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx 0$ yields
$$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+} = \mathbf{A}^{+}$ yields
$$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(x) := f(x) + \varepsilon$ yields
$$=: \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(x - \bar{x})$ by applying it to $(y - \bar{y})$, i.e.

$$\hat{x}(y) := \bar{x} + \bar{\mathbf{K}}(y - \bar{y}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall

$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N-1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields

$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+ \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}, \quad \mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+ \tag{14}$$

$\mathbf{Y}_\text{noisy} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_\text{noisy}\mathbf{Y}_\text{noisy}^\mathsf{T})^+ \tag{15}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1}$ (13)

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+$ (14)

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^+$ (15)

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall

$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields

$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields

$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields

$$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+} = \mathbf{A}^{+}$ yields

$$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(x) := f(x) + \varepsilon$ yields

$$= \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(x - \bar{x})$ by applying it to $(y - \bar{y})$, i.e.

$$\hat{x}(y) := \bar{x} + \bar{\mathbf{K}}(y - \bar{y}) \;\checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+ \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^+ \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^+ \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^+ = \mathbf{A}^+$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1}$ (13)

Then:

$\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$	yields	$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + \mathbf{D}\mathbf{D}^{\mathsf{T}})^{+}$	(14)
$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$	yields	$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+}$	(15)
$\mathbf{X}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$	yields	$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+}$	(16)
$\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+} = \mathbf{A}^{+}$	yields	$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+}$	(17)
$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}) + \varepsilon$	yields	$=: \bar{\nabla}^{-1} f_{\text{noisy}}$.	(18)

(Snyder, 2015)

$\implies$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\implies$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \quad (19)$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall

$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then:

$\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+} \tag{16}$$

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+} = \mathbf{A}^{+}$ yields
$$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}) + \varepsilon$ yields
$$= \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.
$\Longrightarrow$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall
$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + {\scriptstyle (N-1)}\mathbf{R})^{-1} \tag{13}$$

Then:

$\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$ yields
$$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + \mathbf{D}\mathbf{D}^{\mathsf{T}})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\quad \mathbf{Y}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields
$$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{16}$$

$\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+} = \mathbf{A}^{+}$ yields
$$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}) + \varepsilon$ yields
$$=: \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + (N-1)\mathbf{R})^{-1}$ (13)

Then:

$\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$	yields	$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + \mathbf{D}\mathbf{D}^{\mathsf{T}})^{+}$	(14)
$\mathbf{Y}_{\text{noisy}} := \mathbf{Y} + \mathbf{D}$, $\quad \mathbf{Y}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$	yields	$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+}$	(15)
$\mathbf{X}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$	yields	$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+}$	(16)
$\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+} = \mathbf{A}^{+}$	yields	$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+}$	(17)
$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}) + \varepsilon$	yields	$=: \bar{\nabla}^{-1} f_{\text{noisy}}\,.$	(18)

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall

$$\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + (N{-}1)\mathbf{R})^{-1} \tag{13}$$

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^{\mathsf{T}} \approx \mathbf{R}$ yields

$$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}\mathbf{Y}^{\mathsf{T}} + \mathbf{D}\mathbf{D}^{\mathsf{T}})^{+} \tag{14}$$

$\mathbf{Y}_{\text{noisy}} := \mathbf{Y}+\mathbf{D}$, $\mathbf{Y}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields

$$\approx \mathbf{X}\mathbf{Y}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{15}$$

$\mathbf{X}\mathbf{D}^{\mathsf{T}} \approx \mathbf{0}$ yields

$$\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^{\mathsf{T}})^{+} \tag{16}$$

$\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{+} = \mathbf{A}^{+}$ yields

$$= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+} \tag{17}$$

$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}) + \varepsilon$ yields

$$=: \bar{\nabla}^{-1} f_{\text{noisy}} \,. \tag{18}$$

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \tag{19}$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1}$ (13)

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^{+}$ (14)

$\mathbf{Y}_{\text{noisy}} {:=} \mathbf{Y}{+}\mathbf{D}$, $\mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+}$ (15)

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $\approx \mathbf{X}\mathbf{Y}_{\text{noisy}}^\mathsf{T}(\mathbf{Y}_{\text{noisy}}\mathbf{Y}_{\text{noisy}}^\mathsf{T})^{+}$ (16)

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^{+} = \mathbf{A}^{+}$ yields $= \mathbf{X}\mathbf{Y}_{\text{noisy}}^{+}$ (17)

$f_{\text{noisy}}(\boldsymbol{x}) := f(\boldsymbol{x}){+}\varepsilon$ yields $=: \bar{\nabla}^{-1} f_{\text{noisy}}\,.$ (18)

(Snyder, 2015)

$\implies$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_{\text{noisy}}$ "inverts" model + noise.

$\implies$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \checkmark \quad (19)$$

EnKF *is* LLS

What about $\bar{\mathbf{K}}$ itself? Recall $\bar{\mathbf{K}} := \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + (N{-}1)\mathbf{R})^{-1}$ (13)

Then: $\frac{1}{N-1}\mathbf{D}\mathbf{D}^\mathsf{T} \approx \mathbf{R}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}\mathbf{Y}^\mathsf{T} + \mathbf{D}\mathbf{D}^\mathsf{T})^+$ (14)

$\mathbf{Y}_\text{noisy} {:=} \mathbf{Y}{+}\mathbf{D},\quad \mathbf{Y}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $\approx \mathbf{X}\mathbf{Y}^\mathsf{T}(\mathbf{Y}_\text{noisy}\mathbf{Y}_\text{noisy}^\mathsf{T})^+$ (15)

$\mathbf{X}\mathbf{D}^\mathsf{T} \approx \mathbf{0}$ yields $\approx \mathbf{X}\mathbf{Y}_\text{noisy}^\mathsf{T}(\mathbf{Y}_\text{noisy}\mathbf{Y}_\text{noisy}^\mathsf{T})^+$ (16)

$\mathbf{A}^\mathsf{T}(\mathbf{A}\mathbf{A}^\mathsf{T})^+ = \mathbf{A}^+$ yields $= \mathbf{X}\mathbf{Y}_\text{noisy}^+$ (17)

$f_\text{noisy}(\boldsymbol{x}) := f(\boldsymbol{x}){+}\varepsilon$ yields $=: \bar{\nabla}^{-1} f_\text{noisy}\,.$ (18)

(Snyder, 2015)

$\Longrightarrow$ $\bar{\mathbf{K}} = \bar{\nabla}^{-1} f_\text{noisy}$ "inverts" model + noise.

$\Longrightarrow$ Can estimate $(\boldsymbol{x} - \bar{\boldsymbol{x}})$ by applying it to $(\boldsymbol{y} - \bar{\boldsymbol{y}})$, i.e.

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) \;:=\; \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}}) \;\checkmark \tag{19}$$

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \xi$,
so as to "explain" residuals, i.e.

$$\xi \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

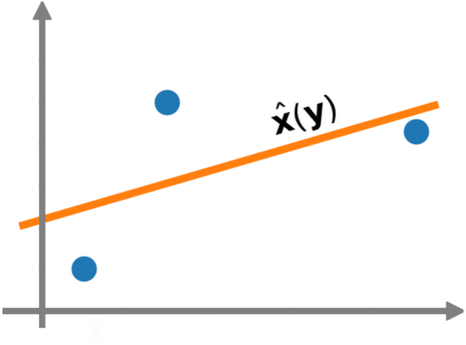
For example, for all n:

$$\xi_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

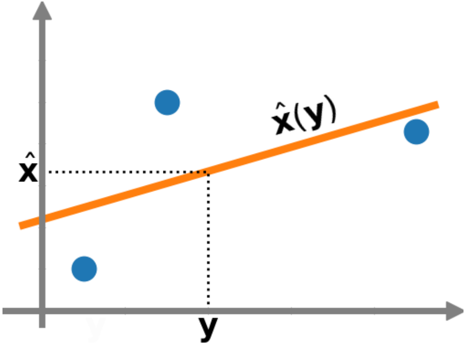
$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \xi_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \; ✓ \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

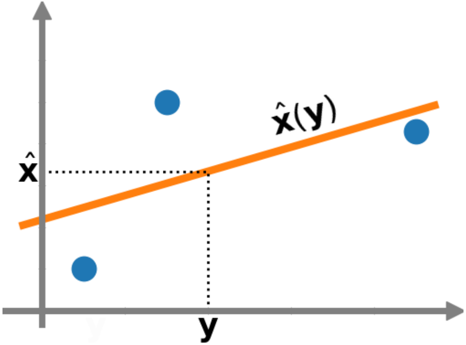
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \;\checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

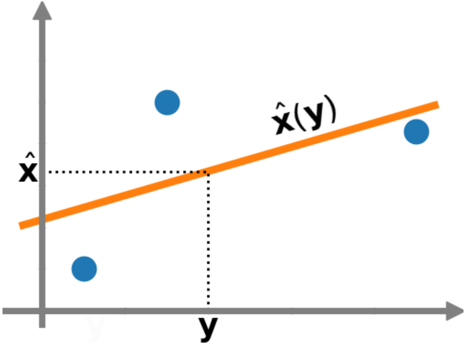
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) \coloneqq \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

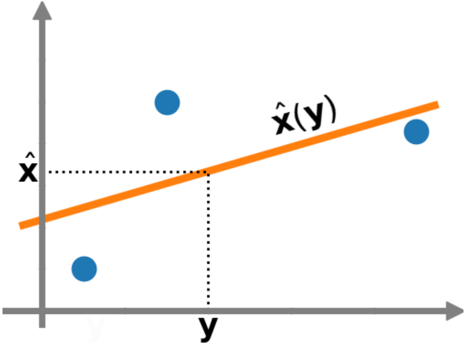
$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \,. \checkmark \tag{22}$$



Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \;\sim\; \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y})\,. \tag{20}$$

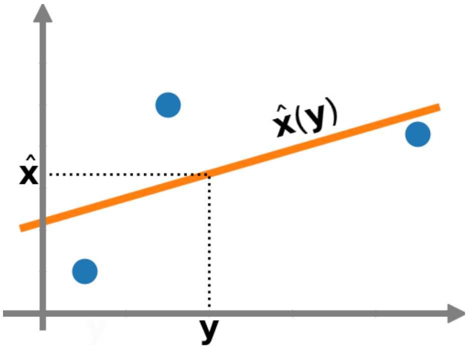
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}})\,. \checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

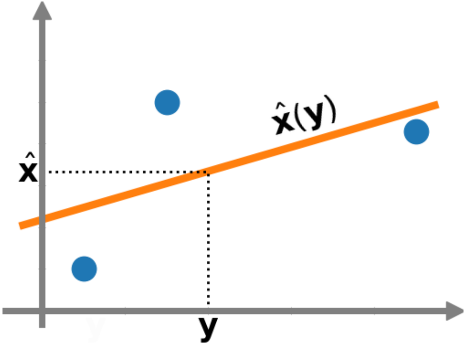
But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$



Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \; \checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

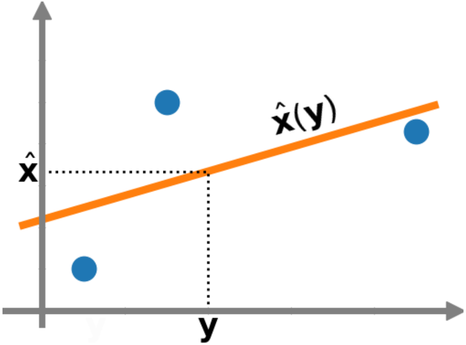
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \;\checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to “explain” residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

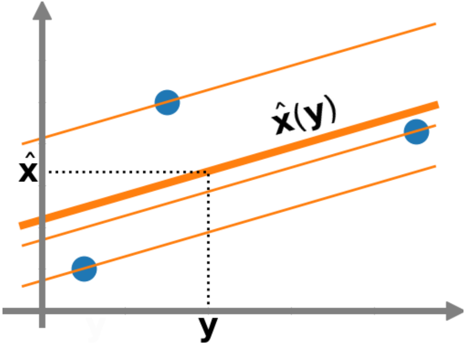
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \;\checkmark \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to “explain” residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

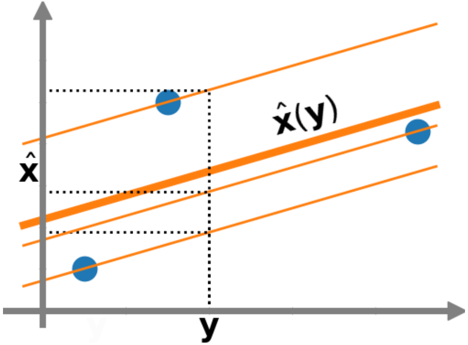
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \; ✓ \tag{22}$$

Alternative: moment matching,
yielding square-root update schemes.



EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

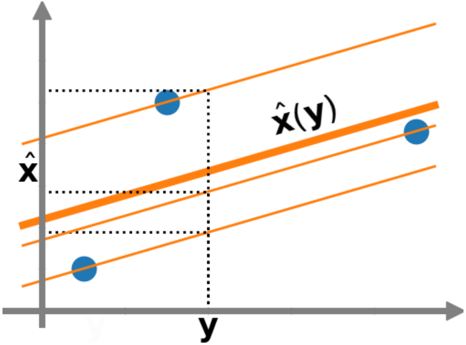
$$\boldsymbol{\xi} \;\sim\; \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y})\,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}})\,. \tag{22}$$



Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

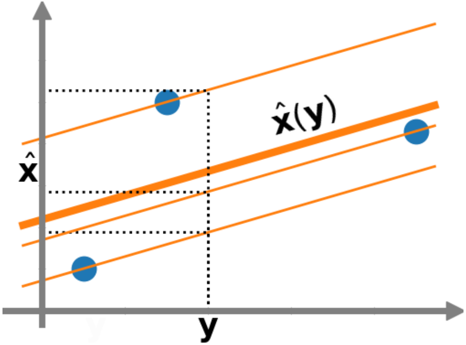
$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y})\,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}})\,. \checkmark \tag{22}$$



Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

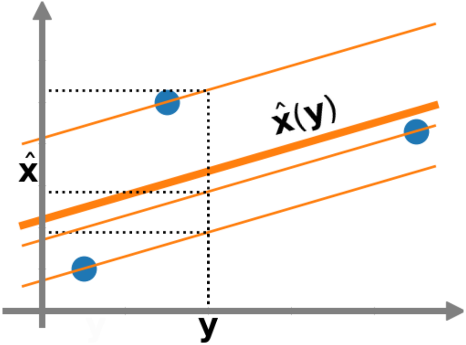
$$\boldsymbol{\xi} \;\sim\; \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y})\,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}})\,.\checkmark \tag{22}$$



Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

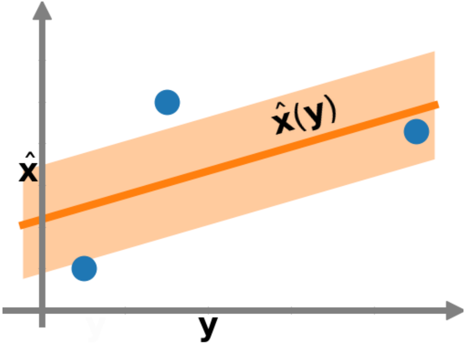
$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \tag{20}$$

For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \tag{21}$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \,. \checkmark \tag{22}$$



Alternative: moment matching,
yielding square-root update schemes.

EnKF *is* LLS (continued)

But $\hat{\boldsymbol{x}}(\boldsymbol{y}) := \bar{\boldsymbol{x}} + \bar{\mathbf{K}}(\boldsymbol{y} - \bar{\boldsymbol{y}})$ only yields the mean update.
What about the full ensemble?

For UQ, add a random error: $\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}$,
so as to "explain" residuals, i.e.

$$\boldsymbol{\xi} \sim \boldsymbol{x} - \hat{\boldsymbol{x}}(\boldsymbol{y}) \,. \qquad (20)$$

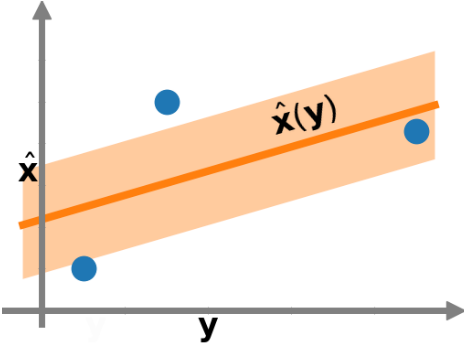
For example, for all n:

$$\boldsymbol{\xi}_n = \boldsymbol{x}_n - \hat{\boldsymbol{x}}(\boldsymbol{y}_n^{\text{noisy}}) \qquad (21)$$

Then

$$\hat{\boldsymbol{x}}(\boldsymbol{y}) + \boldsymbol{\xi}_n = \boldsymbol{x}_n + \bar{\mathbf{K}}(\boldsymbol{y} - \boldsymbol{y}_n^{\text{noisy}}) \,. \checkmark \qquad (22)$$

Alternative: moment matching,
yielding square-root update schemes.



Summary

Summary

Iter. ens
uses LLS

EnKF
uses LLS

EAKF, ETKF
uses LLS

EnKF
is LLS

LLS $\Rightarrow$
avrg. grad

Patrick Nima Raanes, Andreas Størksen Stordal, and Geir Evensen. Revising the stochastic iterative ensemble smoother. *Nonlinear Processes in Geophysics*, 26 (3):325–338, 2019. DOI: 10.5194/npg-26-325-2019.

C. Snyder. Introduction to the Kalman filter. In Eric Blayo, Marc Bocquet, Emmanuel Cosme, and Leticia F. Cugliandolo, editors, *Lecture Notes of the Les Houches School of Physics: Special Issue, 28 May–15 June 2012: Advanced Data Assimilation for Geosciences*, pages 75–120. Oxford University Press, 2015.

Andreas S. Stordal, Slawomir P. Szklarz, and Olwijn Leeuwenburgh. A theoretical look at ensemble-based optimization in reservoir management. *Mathematical Geosciences*, 48(4):399–417, 2016. DOI: 10.1007/s11004-015-9598-6.