# Inverse Problems: A Mathematician's Perspective

Jenn-Nan Wang Seminar@NCU, Mar 17, 2023

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# Introduction



Inverse problems everyday!

- · Medical imaging
- Nondestructive testing
- Radar
- Seismology exploration
- · Remote sensing
- Forensics
- and much more ....

## **General setup**

#### Consider

$$y=G(p),$$

where

$$\left\{ egin{array}{ll} p\in X & ( ext{parameter space}), \ y\in Y & ( ext{data or observation space}) \end{array} 
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and

$$G: X \rightarrow Y$$
 (parameter to data map).

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Inverse problems: given y, determine p.

It is quite often that finding  $G^{-1}$  is impossible.

#### **CT** Scan



The Nobel Prize in Physiology or Medicine 1979 was awarded jointly to Allan M. Cormack and Godfrey N. Hounsfield "for the development of computer assisted tomography"

# X-ray transform



# X-ray transform



 $\ell$  is the red straight line.

 $I_{\text{out}} = I_{\text{in}} \exp(-\int_{\ell} f(x) ds)$ 

 $\textit{I}_{\rm out},\textit{I}_{\rm in}$  are the numbers of photons at the source and the receiver

f(x) is the optical density of the medium

So we can compute the line integral of f(x) along any X-ray by measuring the numbers of photons at the source and the receiver. The question now is to determine f(x) by all its line integrals. In other words, one would like to invert the map:

$$\mathcal{R}: f(x) \to Rf(\ell) = \int_{\ell} f(x) ds,$$

where *Rf* is known to be the Radon transform of *f* in  $\mathbb{R}^2$ .

We can write

$$Rf(\rho,\theta) = \int_{-\infty}^{\infty} f(\rho\cos\theta - s\sin\theta, \rho\sin\theta + s\cos\theta) ds.$$

Let point P = (x, y), define

$$ar{F}_P(q) = rac{1}{2\pi} \int_0^{2\pi} Rf(x\cos heta+y\sin heta+q, heta)d heta$$

then

$$f(P) = -rac{1}{\pi}\int_0^\infty rac{dar{F}_P(q)}{q}.$$

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then

$$f(P) = -\frac{1}{\pi} \int_0^\infty \frac{d\bar{F}_P(q)}{q}.$$

This is the famous inversion formula derived by Radon in 1917.

# Ignored result



#### Johann Radon (1887-1956)



Johann Radon (1887-1956)

Unaware of Radon's result, Cormack reconsidered this reconstruction problem and published two papers in 1963, 1964. It was not until 1970 that Cormack learned that the problem has been solved by Radon.



# Travel time tomography



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To determine the structure of the core by measuring the travel time. This problem can be recasted into a geometry problem. One of them is the problem of determining the Riemannian metric from the lengths of geodesics joining points in the boundary.

# Travel time tomography



To determine the structure of the core by measuring the travel time. This problem can be recasted into a geometry problem. One of them is the problem of determining the Riemannian metric from the lengths of geodesics joining points in the boundary. However, in general, this problem does not have a unique solution.

# **EIT or ERT**



Electrical impedance tompgraphy

## **EIT or ERT**



Electrical impedance tompgraphy



Electrical resistivity tompgraphy

The boundary value problem:

$$\begin{cases} \nabla \cdot (\gamma \nabla u) = 0 \text{ in } \Omega, \\ u = f \text{ on } \partial \Omega, \end{cases}$$

or

$$\begin{cases} \nabla \cdot (\gamma \nabla u) = 0 \text{ in } \Omega, \\ \gamma \frac{\partial u}{\partial \nu} = g \text{ on } \partial \Omega, \int_{\partial \Omega} g d\sigma = 0, \end{cases}$$

where  $\gamma > 0$  is the conductivity function (the inverse of the resistivity), *f* is the voltage potential on the boundary, and *g* is the current on the boundary. Here  $\nu$  is the unit outer normal of  $\partial \Omega$ .

## **Inverse problem**

The problem is to determine  $\gamma$  from the collection of  $\{f, \gamma \frac{\partial u}{\partial \nu}|_{\partial \Omega}\}$ (voltage-current pairs) or  $\{g, u|_{\partial \Omega}\}$  (current-voltage pairs). In the mathematical term: determine  $\gamma$  from

 $\Lambda_{\gamma}$ : voltage  $\rightarrow$  current,  $\Lambda_{\gamma}f = \gamma \frac{\partial u}{\partial \nu}|_{\partial\Omega}$  (Dirichlet-to-Neumann map) or

 $\mathcal{N}_{\gamma}$ : current  $\rightarrow$  voltage,  $\mathcal{N}_{\gamma}g = u|_{\partial\Omega}$  (Neumann-to-Dirichlet map).

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Basic mathematical questions:

- Uniqueness:  $\Lambda_{\gamma_1} = \Lambda_{\gamma_2} \Rightarrow \gamma_1 = \gamma_2$
- Reconstruction: reconstruction formula of determining  $\gamma$  from  $\Lambda_{\gamma}$
- Stability: how error of Λ<sub>γ</sub> affects γ

#### Pioneer



Alberto Calderón (1920-1988)

He studied civil engineering at the University of Buenos Aires and graduated in 1947. He worked at a geophysics research lab at YPF (the state-owned petroleum company) for a few years. A.P. Calderón, ON AN INVERSE BOUNDARY VALUE PROBLEM, in Seminar on Numerical Analysis and its Applications to Continuum Physics, Rio de Janeiro, Editors W.H. Meyer and M.A. Raupp, Sociedade Brasileira de Matematica, (1980). 65-73.

#### Paper

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Alberto Grünbaum

Although the boundary value problem is linear in  $\gamma$ , the problem of determining  $\gamma$  from  $\Lambda_{\gamma}$  is *nonlinear*.

# Calderón's approach

Although the boundary value problem is linear in  $\gamma$ , the problem of determining  $\gamma$  from  $\Lambda_{\gamma}$  is *nonlinear*.

#### Idea: linearization

Consider the nonlinear function y = F(x). Assume that  $y_0 = F(x_0)$ . Then Taylor's formula:

$$y-y_0\approx \nabla F(x_0)(x-x_0),$$

i.e.,

$$x \approx x_0 + (\nabla F(x_0))^{-1}(y - y_0)$$

provided  $\nabla F(x_0)$  is invertible. Also, if  $x_1, x_2$  are near  $x_0$  and  $\nabla F(x_0)$  is invertible, then  $F(x_1) = F(x_2) \Rightarrow x_1 = x_2$ .

#### Energy

Green's identity:

$$\int_{\partial\Omega} \Lambda_{\gamma} f \cdot h d\sigma = \int_{\Omega} \gamma u \cdot v dx := Q_{\gamma}(f, h),$$

where  $v|_{\partial\Omega} = h$ . You can think of  $Q_{\gamma}$  as the energy and

 $\Lambda_{\gamma} \Leftrightarrow Q_{\gamma}.$ 

Then for  $\gamma = \mathbf{1} + \gamma'$ 

$$dQ(1)(\gamma') = \int_{\Omega} \gamma' \nabla u' \cdot \nabla v' dx,$$

where  $\Delta u' = \Delta v' = 0$  in  $\Omega$ , i.e., harmonic functions. Plugging suitable harmonic functions into this formula will give us some information of  $\gamma'$ , a perturbation of the identity conductivity.

# **Global uniqueness**

The linearized map dQ(1) will not provide us any uniqueness result even when dQ(1) is "invertible".

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John Sylvester



Gunther Uhlmann

Proved the uniqueness in 1987:  $\Lambda_{\gamma_1} = \Lambda_{\gamma_2} \Rightarrow \gamma_1 = \gamma_2$ . They introduced a special class of solutions called **complex** geometric optics solutions in the proof. These solutions are also useful in designing a reconstruction algorithm (in theory).

# III-posedness

#### EIT problem is ill-posed in the sense of Hadamard.



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## **III-posedness**

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Hadamard defined that a problem is well-posed if it has existence, uniqueness, and continuous dependence (solution depends on data or on coefficients continuously).

Who cares about the existence and uniqueness?

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In fact, the usual sense of continuous dependence does not hold. That is, let  $(X, |\cdot|_X)$  be the space of  $\gamma$  and  $(Y, |\cdot|_Y)$  be the space of  $\Lambda_{\gamma}$ , where  $|\cdot|_X$  and  $|\cdot|_Y$  are distance functions in Xand Y, respectively. One cannot expect that for any  $\gamma_1, \gamma_2 \in X$ 

$$\operatorname{error}(\Lambda_{\gamma_1}, \Lambda_{\gamma_2}) \to \mathbf{0} \Rightarrow \operatorname{error}(\gamma_1, \gamma_2) \to \mathbf{0},$$

where

$$\begin{cases} \operatorname{error}(\Lambda_{\gamma_1}, \Lambda_{\gamma_2}) = |\Lambda_{\gamma_1} - \Lambda_{\gamma_2}|_Y, \\ \operatorname{error}(\gamma_1, \gamma_2) = |\gamma_1 - \gamma_2|_X. \end{cases}$$
### Stable estimate

But we can find a subspace  $E \subset X$  such that if  $\gamma_1, \gamma_2 \in E$  such that it holds

 $\operatorname{error}(\Lambda_{\gamma_1},\Lambda_{\gamma_2})\to 0 \Rightarrow \operatorname{error}(\gamma_1,\gamma_2)\to 0$ 

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(closely related to the regularization).

In fact, it was proved by Alessandrini that if  $\gamma_1, \gamma_2 \in E$  for some suitable  $E \subset X$ :

$$\operatorname{error}(\gamma_1, \gamma_2) \le C\omega(\varepsilon),$$
 (1)

where  $\varepsilon = \operatorname{error}(\Lambda_{\gamma_1}, \Lambda_{\gamma_2})$ , *C* is some positive constant, and

 $\omega(\varepsilon) \leq |\log \varepsilon|^{-\eta}, \ 0 < \eta < 1.$  (logarithmically stable)

This estimate cannot be improved in general.

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How to improve the stability is probably the most challenging problem in EIT or ERT.

Piecewise constant conductivity:  $\gamma = \sum_{j=1}^{J} c_j \mathbb{1}_{D_j}$ , where  $\mathbb{1}_{D_j}$  is he characteristic function of the region  $D_j$  and  $\Omega = \bigcup_{j=1}^{J} D_j$ . Assume that  $\{D_j\}_{j=1}^{J}$  are known, but  $\{c_j\}_{j=1}^{J}$  are unknown. The determination of  $\{c_j\}_{j=1}^{J}$  by the measurement  $\Lambda_{\gamma}$  is almost *linearly stable*. Piecewise constant conductivity:  $\gamma = \sum_{j=1}^{J} c_j \mathbb{1}_{D_j}$ , where  $\mathbb{1}_{D_j}$  is he characteristic function of the region  $D_j$  and  $\Omega = \bigcup_{j=1}^{J} D_j$ . Assume that  $\{D_j\}_{j=1}^{J}$  are known, but  $\{c_j\}_{j=1}^{J}$  are unknown. The determination of  $\{c_j\}_{j=1}^{J}$  by the measurement  $\Lambda_{\gamma}$  is almost *linearly stable*.

However, if  $\{D_j\}_{j=1}^J$  are unknown, then the determination is still *logarithmically stable*!

Related to the case of piecewise conductivity, we consider the following problem: let  $\gamma = \gamma_0 \mathbb{1}_{\Omega \setminus D} + \gamma_1 \mathbb{1}_D$ . Assume that  $\gamma_0$  is known, but  $\gamma_1$  is unknown. You can regard *D* as the region of an abnormality, e.g., tumor.

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This problem is again logarithmically stable. However, we can observe and also prove mathematically that the reconstruction of D is more stable when D is near the boundary.

## **Stationary equations**

We can consider the Helmholtz type equation

$$\Delta u + k^2 u + q u = 0 \quad \text{in} \quad \Omega,$$

where k is the wave number and q is a potential function. We can study the problem of determining q by the measurements

$$\{u|_{\partial\Omega}, \frac{\partial u}{\partial\nu}|_{\partial\Omega}\}.$$

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For this case, one can observe that the stability estimate tends to a Hölder type as k increases. That is,

$$\operatorname{error}(q_1, q_2) \leq C(k)(\operatorname{error}(\Lambda_{q_1}, \Lambda_{q_2}))^{\alpha} + \underbrace{\operatorname{error term}}_{\downarrow 0 \text{ as } k \to \infty},$$

where  $\alpha \in (0, 1)$ . Stability is increasing if we are prospecting the unknown by the high frequency waves.

## Wave equation

Consider the initial-boundary value problem for the wave equation:

$$\begin{cases} \partial_{tt}^2 v - \Delta v + qv = 0 \quad (x,t) \in \Omega \times (0,T), \\ v(0,x) = 0, \quad \partial_t v(0,x) = 0 \quad x \in \Omega, \\ v(t,x) = f, \quad (x,t) \in \partial\Omega \times (0,T). \end{cases}$$

We can define the measurement  $\Lambda_q^h$ :

$$\Lambda_q^h(f) = \frac{\partial \mathbf{V}}{\partial \nu}\Big|_{\partial \Omega \times (0,T)}$$

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$$\Lambda_q^h(f) = \frac{\partial \mathbf{v}}{\partial \nu} \Big|_{\partial \Omega \times (0,T)}$$

In this problem, the following stability estimate holds

 $\operatorname{error}(q_1, q_2) \leq C(\operatorname{error}(\Lambda^h_{q_1}, \Lambda^h_{q_2}))^{\beta}, \ \beta \in (0, 1).$ 

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For the elliptic (e.g.,  $\Delta u = 0$ ) or parabolic equations (e.g.  $\partial u - \Delta u = 0$ ), the speed of propagation is infinite.

Determine *p* from the observation *y* in y = G(p). Try to solve

$$p = \operatorname*{argmin}_{p \in X} \|y - G(p)\|_Y^2.$$

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Problems:

- Inverse problem is ill-posed. Small perturbations of data will lead to large errors in the determination of *p*. That is, the numerically determined solution is not stable.
- It is difficult to apply a Newton-type scheme since the derivative of *G* is quite often hard to compute.

Solve (Tikhonov's regularization)

$$p = \underset{p \in X}{\operatorname{argmin}} \Big\{ \| y - G(p) \|_{Y}^{2} + \alpha \| p \|_{E}^{2} \Big\}$$

 $E \subset X$ : compact subspace

 $\alpha$ : parameter

Introducing a regularizer can stabilize the problem, but *G* is most likely not convex in *p*. There are many minimizers. Also, the choice of  $\alpha$  is tricky.

## Statistical viewpoint

In practice, there exist measurement errors. Thus, it is more reasonable to consider

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Precisely, let *X*, *Y* be separable Hilbert spaces and  $G: X \to Y$  be a Borel measurable map. Normally,  $\xi$  is a centered Gaussian on *Y*, i.e.  $\xi \sim \mathcal{N}(0, \Gamma)$ , where  $\Gamma$  the covariance operator which is a positive operator of trace class.

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We put a prior on p, i.e. p is a random element on X. It is common to choose  $p \sim \mathcal{N}(\bar{p}, C)$ , the Gaussian with mean  $\bar{p}$  and covariance C.



In most cases, we can express

$$\mathbb{P}(\boldsymbol{\rho}|\boldsymbol{y}) \propto \exp(-\Phi(\boldsymbol{\rho};\boldsymbol{y})).$$

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For the case of  $\xi \sim \mathcal{N}(0, \Gamma)$  and  $u \sim \mathcal{N}(\bar{p}, C)$ ,

$$\Phi(p; y) = \frac{1}{2} \|\Gamma^{-1/2}(y - G(p))\|_Y^2 + \frac{1}{2} \|C^{-1/2}(p - \bar{p})\|_X^2$$

#### Maximum likelihood estimation (MLE):

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#### Minimization with regularization

Both estimations provide point estimators.

Instead of the minimization technique, we can use the posterior distribution to make inference of the parameter.

Let  $\Pi(\cdot|Y)$  be the posterior distribution. The expectation  $\mathbb{E}[\Pi(\cdot|Y)]$  is a natural point estimator of *p*. Formally

$$\mathbb{E}[\Pi(\cdot|Y)] = \int_X p \, \mathrm{d}\Pi(p|Y).$$

This integral can be rigorously defined in Bochner's sense. To be useful, we need to find an effective way to approximate it.

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#### Monte Carlo Integration

Let  $p^{(1)}, \dots, p^{(n)}$  be sampled independently from  $\Pi(\cdot|Y)$ . Then

$$\frac{1}{n}\sum_{k=1}^{n}p^{(k)} \to \mathbb{E}[\Pi(\cdot|Y)]$$

(Law of Large Number)

MCMC algorithms are the most popular and powerful methods to sample probability distributions. However, in dealing with PDE inverse problems, the posteriors in general lie in the infinite dimensional function spaces, it becomes a challenging question to sample such posteriors effectively. MCMC algorithms are the most popular and powerful methods to sample probability distributions. However, in dealing with PDE inverse problems, the posteriors in general lie in the infinite dimensional function spaces, it becomes a challenging question to sample such posteriors effectively.

The *preconditioned Crank-Nicolson algorithm* (pCN) is a method developed to sample distributions at high dimensions. The pCN method is a Metropolis-type algorithm. Most importantly, the pCN algorithm has dimension-independent sampling efficiency.

Kalman filter method can also be used to study inverse problems. As before, let  $G: X \rightarrow Y$  be the forward map

y = G(q).

Let  $Z = X \times Y$  and the map  $\Theta : Z \to Z$  defined by

$$\Theta(z) = \begin{pmatrix} q \\ G(q) \end{pmatrix}$$
 for  $z = \begin{pmatrix} q \\ p \end{pmatrix}$ , where  $p \in Y$ .

We consider the artificial dynamics given by

$$z_{\ell+1} = \Theta(z_{\ell}), \quad \ell = 0, 1, 2, \cdots.$$
 (2)

Associated to the dynamical equation is the observation equation

$$y_{\ell+1} = Hz_{\ell+1} + \eta_{\ell+1}, \tag{3}$$

where  $H: Z \to Y$  is the projection operator given by  $H = \begin{pmatrix} 0 \\ I \end{pmatrix}$ and  $\eta_1, \eta_2, \cdots$  are independent Gaussian random elements on *Y*.
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The dynamical system (2) gives rises to a prediction step and the observation equation (3) provides a correction step.

## **EnKF** : initial ensemble

Initial ensemble:  $\{z_0^{(j)}\}_{j=1}^J$  are determined by the prior knowledge of q. Let  $\mu_0$  be the prior distribution of q, the initial ensemble consists of  $\{q_0^{(j)}\}_{j=1}^J$ , which are i.i.d. samples of  $\mu_0$ . We now define the space of initial ensemble

$$\mathcal{A} = \{q_0^{(j)}\}_{j=1}^J.$$

Alternatively, if  $\mu_0 \sim \mathcal{N}(\bar{q}, C)$ , we can consider  $q_0^{(j)} = \bar{q} + \sqrt{\alpha_j}\zeta_j$ ,  $j \leq J$ , where  $(\alpha_j, \zeta_j)$  are eigenpairs of *C*. This is known as Karhunen-Loéve basis.

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Initial ensemble:  $\{z_0^{(j)}\}_{j=1}^J$  are determined by the prior knowledge of q. Let  $\mu_0$  be the prior distribution of q, the initial ensemble consists of  $\{q_0^{(j)}\}_{j=1}^J$ , which are i.i.d. samples of  $\mu_0$ . We now define the space of initial ensemble

$$\mathcal{A} = \{q_0^{(j)}\}_{j=1}^J.$$

Alternatively, if  $\mu_0 \sim \mathcal{N}(\bar{q}, C)$ , we can consider  $q_0^{(j)} = \bar{q} + \sqrt{\alpha_j}\zeta_j$ ,  $j \leq J$ , where  $(\alpha_j, \zeta_j)$  are eigenpairs of *C*. This is known as Karhunen-Loéve basis.

Assume that the observational data *y* is given by the "ground truth"  $q^{\dagger} \in X$  with a measurement noise, i.e.,

$$y = G(q^{\dagger}) + \eta^{\dagger}$$

where  $\eta^{\dagger}$  denotes the measurement noise.

# Algorithm

#### Algorithm. Iterative EnKF.

Let the initial ensemble  $\{q_0^{(j)}\}_{j=1}^J$  have been chosen. Denote

$$p_0^{(j)} = G(q_0^{(j)}) ext{ and } z_0^{(j)} = egin{pmatrix} q_0^{(j)} \ p_0^{(j)} \end{pmatrix}. ext{ For } \ell = 0, 1, 2, \cdots.$$

(1) **Prediction step**. Propagate the ensemble particles by the dynamical system (2):

$$\widehat{z}_{\ell+1}^{(j)} = \Theta(z_{\ell}^{(j)}), \ \ j = 1, \cdots, J.$$
 (4)

Sample mean:  $\overline{z}_{\ell+1} = \frac{1}{J} \sum_{j=1}^{J} \widehat{z}_{\ell+1}^{(j)}$ Sample covariance:

$$C_{\ell+1} = \frac{1}{J-1} \sum_{j=1}^{J} \widehat{z}_{\ell+1}^{(j)} (\widehat{z}_{\ell+1}^{(j)})^T - \overline{z}_{\ell+1} (\overline{z}_{\ell+1})^T.$$

(2) **Analysis step**. Here we would like to update the ensemble particles that were obtained in (1) by the observational data. We first define the Kalman gain  $K_{\ell}$  by

$$K_{\ell+1} = C_{\ell+1} H^* (HC_{\ell+1} H^* + \Gamma)^{-1},$$

where  $H^* = (0, I_N)$ . Then each ensemble particle is updated as follows:

$$\begin{aligned} z_{\ell+1}^{(j)} = & \widehat{z}_{\ell+1}^{(j)} + K_{\ell+1}(y_{\ell+1}^{(j)} - H\widehat{z}_{\ell+1}^{(j)}) \\ = & (I - K_{\ell+1}H)\widehat{z}_{\ell+1}^{(j)} + K_{\ell+1}y_{\ell+1}^{(j)}, \end{aligned}$$

where

$$y_{\ell+1}^{(j)} = y + \eta_{\ell+1}^{(j)},$$

where  $\eta_{\ell+1}^{(j)}$  are i.i.d. with  $\eta_{\ell+1}^{(j)} \sim \eta_{\ell+1}$  for  $j = 1, \cdots, J$ .

(3) Compute the updated sample mean

$$q_{\ell+1} = rac{1}{J} \sum_{j=1}^{J} H^{\perp} z_{\ell+1}^{(j)},$$

where  $H^{\perp} = (I, 0)$ .

(3) Compute the updated sample mean

$$q_{\ell+1} = \frac{1}{J} \sum_{j=1}^{J} H^{\perp} z_{\ell+1}^{(j)},$$

where  $H^{\perp} = (I, 0)$ .

Subspace invariance property:  $\{q_{\ell}^{(j)}\}_{j=1}^{J} \in \mathcal{A} \text{ for all } \ell \in \mathbb{N}.$ 

(3) Compute the updated sample mean

$$q_{\ell+1} = \frac{1}{J} \sum_{j=1}^{J} H^{\perp} z_{\ell+1}^{(j)},$$

where  $H^{\perp} = (I, 0)$ .

Subspace invariance property:  $\{q_{\ell}^{(j)}\}_{j=1}^{J} \in \mathcal{A}$  for all  $\ell \in \mathbb{N}$ .

- Interesting questions:
  - Choice of initial ensemble
  - Stopping criteria
  - Convergence theory

# Thank you for your attention