

Constrained Denoising, Empirical Bayes and Optimal Transport

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May 14, 2026

¹Supported by grants DMS-2311062 and DMS-2515520



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García Trillos, N. and **Sen, B.** (2024). A New Perspective On Denoising Based On Optimal Transport. *Information and Inference*, **13**.

<https://arxiv.org/abs/2312.08135>

Jaffe, A., Ignatiadis, N., and **Sen, B.** (2025+). Constrained Denoising, Empirical Bayes and Optimal Transport. *JRSS-B* (under revision)

<https://arxiv.org/abs/2506.09986>

Denosing: a simple latent variable model

- **Model:** $(Z, \Theta) \sim P_{Z, \Theta}$ where

$$Z \mid \Theta = \theta \sim p(\cdot \mid \theta), \quad \text{and} \quad \Theta \sim G^*$$

- **Observation:** $Z \in \mathbb{R}^d$
- **Latent variable:** $\Theta \in \Omega \subset \mathbb{R}^m$ (unobserved)

- $\{p(\cdot \mid \theta)\}_{\theta \in \Omega}$ — pdf/pmf of **known** parametric family
- Examples: $N(\theta, \Sigma)$ (Σ known), $\text{Poisson}(\theta)$, $N(0, \theta)$, $\text{Uniform}(0, \theta)$...

- G^* : Distribution of the **latent variable** (**unknown**)

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Data: Z_1, \dots, Z_n from the above model

Goal: **Denoise** $\{Z_i\}_{i=1}^n$, i.e., **predict** the latent/unobserved $\{\Theta_i\}_{i=1}^n$

Oracle Bayes estimator under squared error loss

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Goal: Given Z predict Θ

Oracle Bayes estimator

A standard approach is to consider:

$$\inf_{\delta: \mathbb{R}^d \rightarrow \mathbb{R}^m} \mathbb{E}_{(Z, \Theta) \sim P_{Z, \Theta}} [\|\delta(Z) - \Theta\|^2],$$

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$\bar{\theta}(Z)$: **Optimal** in terms of minimizing the **(Bayes) risk** w.r.t. **squared loss**

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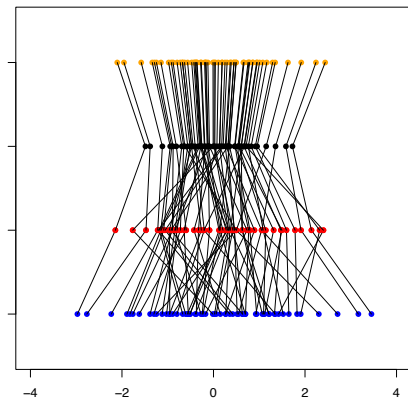
Empirical Bayes: Estimate $\bar{\theta}(\cdot)$ by $\hat{\theta}(\cdot)$ (as G^* is usually **unknown**)

References: Robbins (1951, 1956), Dyson (1926), Jiang & Zhang (2009), Efron (2019)

Drawbacks of $\bar{\theta}(\cdot)$: denoising an ensemble

Example 1: (Normal location mixture) $\{(\Theta_i, Z_i)\}_{i=1}^n$ i.i.d. (here $n = 60$):

$$Z \mid \Theta = \theta \sim N(\theta, 1), \theta \in \mathbb{R}; \quad \Theta \sim G^* \equiv N(0, 1)$$

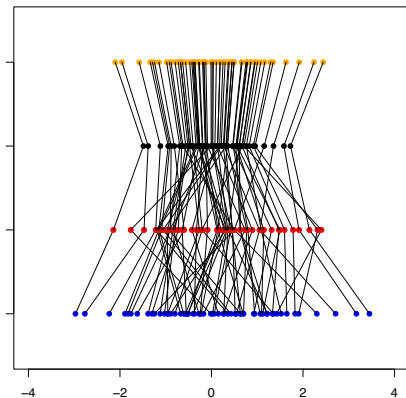


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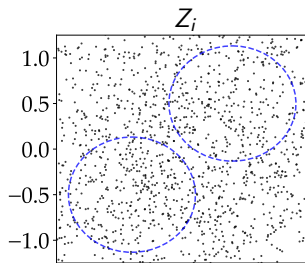
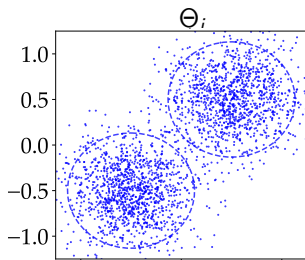
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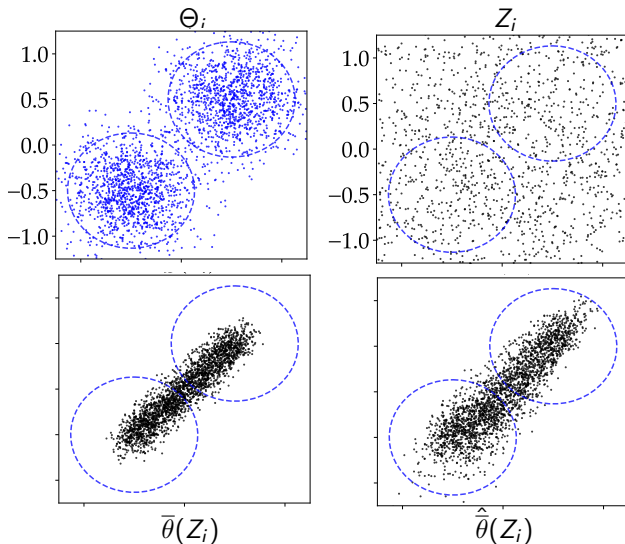
Overshrunk! Observe that $\bar{\theta}(Z) = \frac{1}{2}Z \sim N(0, \frac{1}{2})$



Observations. Latent variables. Bayes estimator. OT-based denoiser.

In general: $\text{Var}(\Theta) = \text{Var}(\bar{\theta}(Z)) + \mathbb{E}[\text{Var}(\Theta \mid Z)] \geq \text{Var}(\bar{\theta}(Z))$





Empirical Bayes: Estimate $\bar{\theta}(\cdot)$ by $\hat{\theta}(\cdot)$ (as G^* is usually unknown)

Posterior means **shrink** the ensemble

Some history

- Astronomers use the **empirical distribution** of Bayes estimates $\hat{\theta}(Z_1), \dots, \hat{\theta}(Z_n)$ and interpret it as an **improved estimate** of the distribution of $\Theta_1, \dots, \Theta_n$ (Loredo, 2007)
- The distribution of $\{\hat{\theta}(Z_i)\}_{i=1}^n$ is **NOT** a good estimator of G^*
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- **Statistics literature**: Various ways to formalize this idea have been taken up in some existing works, e.g., **Louis (1984)**, **Ghosh (1992)**, **Shen and Louis (1998)**, **Ghosh and Maiti (1999)**, ...

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- **Goal:** Estimate/Predict $\Theta_1, \dots, \Theta_n \in \mathbb{R}^m$
- **Original problem** targets the oracle Bayes estimator $\bar{\theta}(\cdot)$:

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$$\begin{cases} \text{minimize} & \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\delta(Z_i) - \Theta_i\|^2 \right] \\ \text{over} & \delta : \mathbb{R}^d \rightarrow \mathbb{R}^m \end{cases}$$

- $\bar{\theta}(\cdot)$ overshrinks!

Question: How to rectify this drawback of $\bar{\theta}(\cdot)$?

Our proposal: OT-based Denoiser

Add constraints:

$$\left\{ \begin{array}{l} \text{minimize} \quad \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\delta(Z_i) - \Theta_i\|^2 \right] \\ \text{over} \quad \delta : \mathbb{R}^d \rightarrow \mathbb{R}^m \\ \text{with} \quad \delta(Z) \stackrel{\mathcal{D}}{=} \Theta \end{array} \right.$$

i.e., the denoised ensemble has the **same distribution** as the **latent ensemble**

Our proposal: Variance constrained denoiser

Add constraints:

$$\left\{ \begin{array}{ll} \text{minimize} & \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\delta(Z_i) - \Theta_i\|^2 \right] \\ \text{over} & \delta : \mathbb{R}^d \rightarrow \mathbb{R}^m \\ \text{with} & \mathbb{E}[\delta(Z)] = \mathbb{E}[\Theta] \\ \text{and} & \text{Var}(\delta(Z)) = \text{Var}(\Theta) \end{array} \right.$$

Our proposal: General constrained denoiser

Fix a **linearly independent** set of functions $\phi_1, \dots, \phi_k : \mathbb{R}^m \rightarrow \mathbb{R}$

Add constraints:

$$\left\{ \begin{array}{ll} \text{minimize} & \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\delta(Z_i) - \Theta_i\|^2 \right] \\ \text{over} & \delta : \mathbb{R}^d \rightarrow \mathbb{R}^m \\ \text{with} & \mathbb{E}[\phi_\ell(\delta(Z))] = \mathbb{E}[\phi_\ell(\Theta)] \quad \text{for all } 1 \leq \ell \leq k \end{array} \right.$$

Add constraints:

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Questions

- **Oracle solution?** (i.e., when G^* is **known**)

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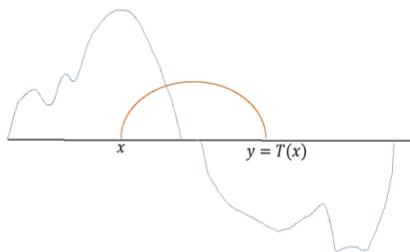
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Questions

- **Oracle solution?** (i.e., when G^* is **known**)
- **Empirical Bayes approximation?**

Optimal Transport (OT): Monge's problem

What is the cheapest way to **transport** a pile of sand to cover a sinkhole?



- $\nu, \tilde{\nu}$: two probability measures on Polish spaces \mathcal{X} and \mathcal{Y}
- $c(x, y)$: **cost** of **transporting** x to y (e.g., $c(x, y) = \|x - y\|^2$)
- **Goal:**
$$\inf_{T: T_{\#}\nu = \tilde{\nu}} \mathbb{E}_{\nu}[c(X, T(X))]$$
- T **transports** ν to $\tilde{\nu}$: $T_{\#}\nu = \tilde{\nu}$ (i.e., $T(X) \sim \tilde{\nu}$ when $X \sim \nu$)

Let ν and $\tilde{\nu}$ be two distributions over \mathbb{R}^m with finite second moments

Kantorovich relaxation:

$$W_2^2(\nu, \tilde{\nu}) := \min_{\pi \in \Gamma(\nu, \tilde{\nu})} \int \int \|x - y\|^2 d\pi(x, y), \quad (1)$$

where $\Gamma(\nu, \tilde{\nu})$ denotes set of all joint distributions on $\mathbb{R}^m \times \mathbb{R}^m$ with marginals ν and $\tilde{\nu}$. (1) is a linear program.

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Brenier's theorem

Suppose that ν has a Lebesgue density. Then,

- \exists a convex function ψ whose gradient $\nabla\psi$ pushes ν forward to $\tilde{\nu}$.
- $\nabla\psi$ (ν -a.e.) uniquely minimizes Monge's problem, i.e.,

$$\nabla\psi = \operatorname{argmin}_{T: T\# \nu = \tilde{\nu}} \int \|x - T(x)\|^2 d\nu(x)$$

- The coupling^a $(\operatorname{Id} \times \nabla\psi)\# \nu$ uniquely minimizes (1).

^aThe map $(\operatorname{Id} \times T) : \mathbb{R}^m \rightarrow \mathbb{R}^m \times \mathbb{R}^m$ is defined as $(\operatorname{Id} \times T)(x) = (x, T(x))$.

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 - If T is a solution to the Monge problem, then the distribution of $(X, T(X))$ for $X \sim \nu$ is a solution to the Kantorovich problem.

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 - If π is a solution to the Kantorovich problem, then the *barycentric projection*

$$T(x) := \mathbb{E}_\pi[X' \mid X = x]$$

for $(X, X') \sim \pi$ is a solution to the Monge problem

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Thus, the Monge problem can be solved via the Kantorovich problem

1. Existence & Characterization of OT-based Denoiser

- **Model:** $Z \mid \Theta = \theta \sim p(\cdot \mid \theta)$, and $\Theta \sim G^*$
- **Problem:** $\inf_{\delta: \delta_{\#} \mu = G^*} \mathbb{E} [\|\delta(Z) - \Theta\|^2]$ ($Z \sim \mu, \Theta \sim G^*$)
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- **Equivalent problem:** $\inf_{\delta: \delta_{\#} \mu = G^*} \mathbb{E}_{Z \sim \mu} [\|\delta(Z) - \bar{\theta}(Z)\|^2]$ (**)

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OT formulation

- Observe: $(\star\star) \equiv \inf_{\delta: \delta_{\#} \mu = G^*} \mathbb{E}_{Z \sim \mu} [c_{G^*}(Z, \delta(Z))]$ where

$$c_{G^*}(z, \vartheta) := \|\vartheta - \bar{\theta}(z)\|^2$$

- The **cost function** $c_{G^*}(\cdot, \cdot)$ **depends** on G^* via $\bar{\theta}(\cdot) = \mathbb{E}_{G^*}[\Theta \mid Z = \cdot]$

Theorem 1 (García Trillos and S., 2024)

Suppose $(Z, \Theta) \sim P_{Z, \Theta}$ with marginals $\Theta \sim G^*$ and $Z \sim \mu$. Under suitable assumptions,

- 1 there exists μ -a.e. **unique** solution $\delta^*(\cdot)$:

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- 2 Furthermore, $\delta^*(\cdot)$ can be written as, for some **convex** function φ ,

$$\delta^*(z) = \nabla \varphi^*(\bar{\theta}(z)), \quad \text{for } z \in \mathbb{R}^d,$$

where $\nabla \varphi^*$ is the OT map from $\bar{\theta}_{\#} \mu$ to G^* .

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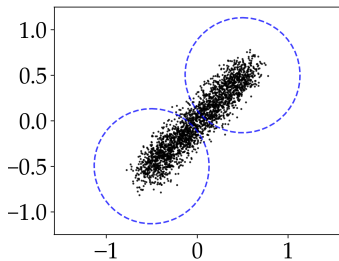
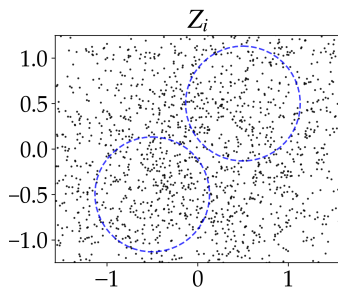
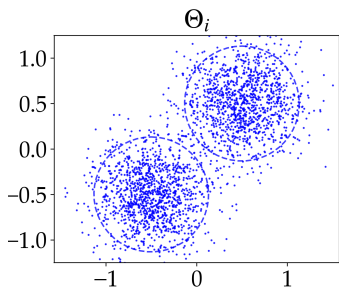
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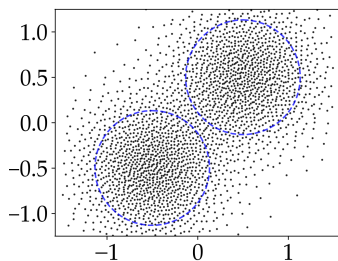
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- 3 Note: $\delta^*(z) = \mathbb{E}_{\pi^*}[\vartheta \mid Z = z]$ where

$$\pi^* = \operatorname{argmin}_{\pi \in \Gamma(\mu, G^*)} \mathbb{E}_{\pi} [\|\vartheta - \bar{\theta}(Z)\|^2]$$



$\bar{\theta}(Z_i)$ (posterior means)



$\delta^*(Z_i)$ (OT-based denoiser)

OT restores the latent distribution while staying close to posterior means

2. Finite Sample Denoising via Empirical Bayes

Model: $Z | \Theta = \theta \sim p(\cdot | \theta)$, and $\Theta \sim G^*$

(Oracle) OT-based denoiser:

$$\delta^* \equiv \operatorname{argmin}_{\delta: \mathbb{R}^d \rightarrow \mathbb{R}^m} \mathbb{E}_{G^*} [\|\delta(Z) - \Theta\|^2] \quad \text{s.t. } \delta(Z) \sim G^*$$

The proposal so far **explicitly** uses G^* to define **OT-based denoiser**

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Question: How would one **estimate** the OT-based denoiser δ^* from i.i.d. data Z_1, \dots, Z_n , if G^* is **unknown**?

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Leads us to problems in **deconvolution** (estimation of G^*) and/or **empirical Bayes** (estimation of the oracle posterior means) methods

An empirical Bayes approach to estimating G^*

- Observe Z_1, \dots, Z_n i.i.d. from model: $Z \mid \Theta = \theta \sim p(\cdot \mid \theta)$, $\Theta \sim G^*$
- Assume here that G^* is **unknown** and belongs to a family \mathcal{P}
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- **Maximum likelihood (ML)** estimator: $\hat{G} \in \mathcal{P}$ maximizes the **marginal (log)-likelihood** of the observations $(Z_i)_{i=1}^n$, i.e.,

$$\hat{G} \in \underset{G \in \mathcal{P}}{\operatorname{argmax}} \sum_{i=1}^n \log f_G(Z_i)$$

- **References**: Robbins (1950), Kiefer and Wolfowitz (1956), ..., Lindsay (1995), Jiang-Zhang (2009), Koenker-Mizera (2014), ...

Recall: OT-based denoiser $\delta^*(z) = \mathbb{E}_{\pi^*}[\vartheta \mid Z = z]$ where

$$\pi^* = \operatorname{argmin}_{\pi \in \Gamma(\mu, G^*)} \int \|\bar{\theta}(z) - \vartheta\|^2 d\pi(z, \vartheta)$$

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- 2 Solve the empirical OT problem:

$$\hat{\pi} \in \operatorname{argmin}_{\pi \in \Gamma(\mu_n, \hat{\mathcal{G}})} \int \|\hat{\theta}(z) - \vartheta\|^2 d\pi(z, \vartheta),$$

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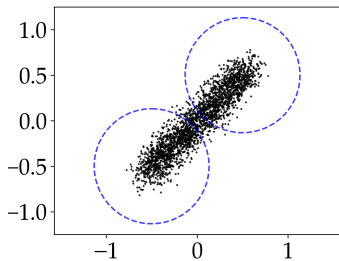
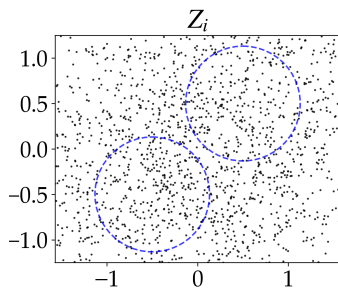
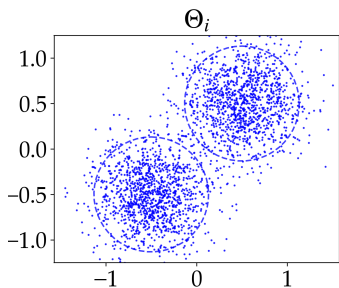
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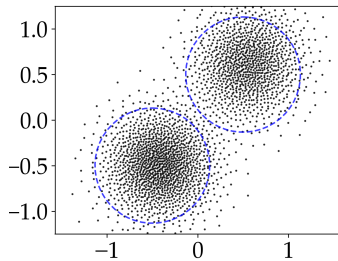
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- 3 Estimate $\delta^*(Z_i)$ by the barycentric projection

$$\hat{\delta}(Z_i) := \mathbb{E}_{\hat{\pi}}[\vartheta \mid Z = Z_i] \quad \text{where} \quad (Z, \vartheta) \sim \hat{\pi}$$



$\bar{\theta}(Z_i)$ (posterior means)



$\hat{\delta}(Z_i)$ (OT-based denoiser)

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Assumptions

$$\frac{1}{n} \sum_{i=1}^n \|\hat{\theta}(Z_i) - \bar{\theta}(Z_i)\|^2 = O_{\mathbb{P}}(r_n), \quad W_2^2(\hat{G}, G^*) = O_{\mathbb{P}}(q_n)$$

Theorem [Jaffe, Ignatiadis, S. (2025+)]

Under suitable assumptions, as $n \rightarrow \infty$, we have:

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The rate of convergence is determined by whichever of **unconstrained Bayes denoising** and **deconvolution** is slower

3. Variance-Constrained Denoising

Variance-constrained denoiser

- **Model:** $Z \mid \Theta = \theta \sim p(\cdot \mid \theta)$, and $\Theta \sim G^*$
- **Data:** $Z \in \mathbb{R}^d$; **latent variable:** $\Theta \in \Omega \subset \mathbb{R}^m$
- Consider the following optimization problem:

$$\begin{cases} \min_{\delta: \mathbb{R}^d \rightarrow \mathbb{R}^m} & \mathbb{E} [\|\delta(Z) - \Theta\|^2] \\ \text{s.t.} & \mathbb{E}[\delta(Z)] = \mathbb{E}[\Theta] \\ \text{and} & \text{Var}(\delta(Z)) = \text{Var}(\Theta) \end{cases}$$

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- **Idea:** Minimize the **risk** while ensuring that the denoiser $\delta(Z)$ has **first** and **second** moments **matching** that of the latent variable Θ
- **Recall:** $\text{Var}(\Theta) = \text{Var}(\bar{\theta}(Z)) + \mathbb{E}[\text{Var}(\Theta \mid Z)] \geq \text{Var}(\bar{\theta}(Z))$

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Variance constrained denoiser: any solution $\delta_{VC}(\cdot)$ to $(*)$

Questions: Existence of solutions? Characterization?

Model: $Z \mid \Theta = \theta \sim p(\cdot \mid \theta)$, and $\Theta \sim G^*$

Variance-constrained denoiser $\delta_{VC}(z)$ solves:

$$\begin{cases} \min_{\delta: \mathbb{R}^m \rightarrow \mathbb{R}^m} & \mathbb{E} [\|\delta(Z) - \Theta\|^2] \\ \text{s.t.} & \mathbb{E}[\delta(Z)] = \mathbb{E}[\Theta] \\ \text{and} & \text{Var}(\delta(Z)) = \text{Var}(\Theta) \end{cases}$$

Theorem [Jaffe, Ignatiadis, S. (2025+)]

The **variance-constrained Bayes denoiser** is given by:

$$\delta_{VC}(z) := t_{\text{Var}(\bar{\theta}(z))}^{\text{Var}(\Theta)} (\bar{\theta}(z) - \mathbb{E}[\Theta]) + \mathbb{E}[\Theta],$$

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(connection to **Gaussian OT**) where for p.d. matrices A, B ,

$$t_A^B := A^{-1/2} \left(A^{1/2} B A^{1/2} \right)^{\frac{1}{2}} A^{-1/2},$$

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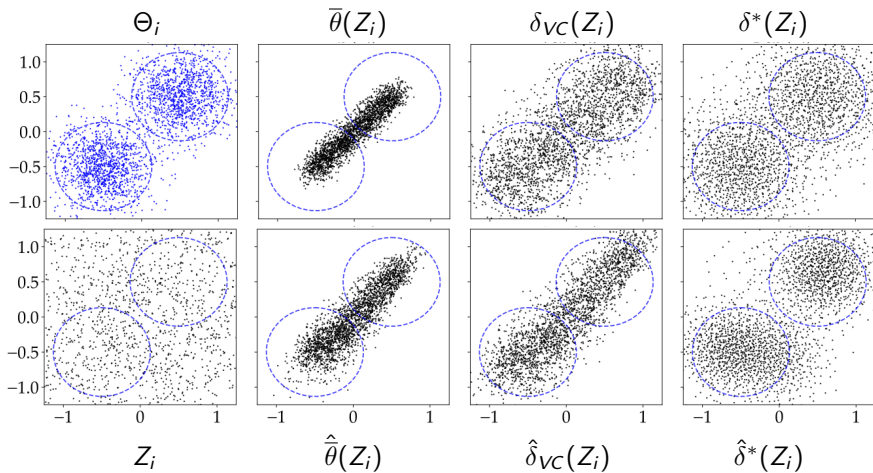
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Question: Given data Z_1, \dots, Z_n , how to **estimate** δ_{VC} ?

Algorithm: Gaussian Noise + NP prior

Model: $Z \mid \Theta = \theta \sim N(\theta, \Sigma)$, and $\Theta \sim G^*$ (Σ known)

Recall: $\delta_{VC}(z) := t_{\text{Var}(\bar{\theta}(z))}^{\text{Var}(\Theta)}(\bar{\theta}(z) - \mathbb{E}[\Theta]) + \mathbb{E}[\Theta]$



$\hat{\delta}^*$ is obtained from **smooth NPMLE** [Magder-Zeger,1996; Kim-S.,2026)]

$\hat{\delta}_{VC}$ partially restore **spread**; $\hat{\delta}^*$ restores **shape**

General constrained denoising

- Fix a **linearly independent** set of functions $\phi_1, \dots, \phi_k : \mathbb{R}^m \rightarrow \mathbb{R}$
- We consider the problem

$$\begin{cases} \text{minimize} & \mathbb{E} [\|\delta(Z) - \Theta\|^2] \\ \text{over} & \delta : \mathbb{R}^d \rightarrow \mathbb{R}^m \\ \text{with} & \mathbb{E}[\phi_\ell(\delta(Z))] = \mathbb{E}[\phi_\ell(\Theta)] \quad \text{for all } 1 \leq \ell \leq k \end{cases} \quad (2)$$

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Under suitable assumptions, (2) has a **unique** solution δ_{GC} .

$\hat{\delta}_{GC}$: **consistent** estimator of δ_{GC} from solving a **sample** version of (2)

- 1 The OT-based denoiser δ^* can rectify drawbacks of posterior mean
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- 4 Framework can be extended to study general constrained denoiser

Thank you for your attention!

Questions?

Original problem

$$\min \mathbb{E} [\|\delta(Z) - \bar{\theta}(Z)\|^2]$$

over $\delta : \mathbb{R}^d \rightarrow \mathbb{R}^m$

s.t. $\mathbb{E}[\delta(Z)] = \mathbb{E}[\Theta]$
and $\text{Var}(\delta(Z)) = \text{Var}(\Theta)$

Gaussian OT

$$\min_{\pi} \mathbb{E}_{\pi} [\|U - V\|^2]$$

jointly Gaussian $(U, V) \sim \pi$

$$U \sim N(\mathbb{E}[\Theta], \text{Var}(\Theta))$$

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RHS \leq LHS

For any δ feasible for **LHS**, consider

$$\begin{pmatrix} U \\ V \end{pmatrix} \sim N \left(\begin{pmatrix} \mathbb{E}[\Theta] \\ \mathbb{E}[\Theta] \end{pmatrix}, \begin{pmatrix} \text{Var}(\Theta) & \text{Cov}(\delta(Z), \bar{\theta}(Z)) \\ \text{Cov}(\bar{\theta}(Z), \delta(Z)) & \text{Var}(\bar{\theta}(Z)) \end{pmatrix} \right)$$

Further, $\mathbb{E} [\|\delta(Z) - \bar{\theta}(Z)\|^2] = \mathbb{E} [\|U - V\|^2]$

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For strictly p.d. matrices A, B , $t_A^B := A^{-1/2} (A^{1/2} B A^{1/2})^{\frac{1}{2}} A^{-1/2}$,
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Then,

$$\text{LHS} \leq \mathbb{E} [\|\delta(Z) - \bar{\theta}(Z)\|^2] = \mathbb{E} [\|T(V) - V\|^2] = \text{RHS}$$