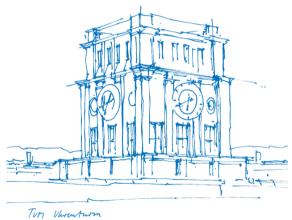


# **Robust Score Matching** Using the geometric median

#### **Bichard Schwank**

Mathematical Statistics Department of Mathematics Technical University of Munich

September 1<sup>st</sup>, 2025



#### **Outline**



- Score Matching using the Geometric Median (AISTATS 2025)
- Some phenomena in high dimensions (arXiv:2508.12926)

#### Setup



#### Score Matching



$$\nabla \log(c \cdot p(x)) = \nabla \log(p(x))$$

#### Robustness





#### Exponential family/ Graphical model



## **Exponential family score matching**



Density model:  $p(\mathbf{x} \mid \boldsymbol{\theta}) = \exp\left(\boldsymbol{\theta}^{\top}\mathbf{t}(\mathbf{x}) - a(\boldsymbol{\theta}) + b(\mathbf{x})\right)$  with  $\mathbf{x} \in \mathcal{X}$  and parameter  $\boldsymbol{\theta} \in \mathbb{R}^r$ .

$$\begin{aligned} \boxed{\boldsymbol{\theta}_0} &= \operatorname{argmin}_{\boldsymbol{\theta}} & \frac{1}{2} \operatorname{E}_{\mathbf{x} \sim p(\cdot \mid \boldsymbol{\theta}_0)} \left[ \| \nabla_{\mathbf{x}} \log(p(\mathbf{x} \mid \boldsymbol{\theta})) - \nabla_{\mathbf{x}} \log(p(\mathbf{x} \mid \boldsymbol{\theta}_0)) \|^2 \right] \\ &= \operatorname{argmin}_{\boldsymbol{\theta}} & \frac{1}{2} \operatorname{E}_{\boldsymbol{\theta}_0} \left[ \| \nabla_{\mathbf{x}} \log(p(\mathbf{x} \mid \boldsymbol{\theta})) \|^2 \right] + \operatorname{E}_{\boldsymbol{\theta}_0} \left[ \Delta_{\mathbf{x}} \log(p(\mathbf{x} \mid \boldsymbol{\theta})) \right] \end{aligned}$$

$$=: \operatorname{argmin}_{\boldsymbol{\theta}} \ \ \tfrac{1}{2} \boldsymbol{\theta}^T \ \operatorname{E}_{\boldsymbol{\theta}_0}[\, \boldsymbol{\Gamma}(\mathbf{x}) \,] \, \boldsymbol{\theta} + \boldsymbol{\theta}^T \ \operatorname{E}_{\boldsymbol{\theta}_0}[\, \mathbf{g}(\mathbf{x}) \,]$$

for some  $\Gamma(\mathbf{x}) \in \mathbb{R}^{r \times r}$  and  $\mathbf{g}(\mathbf{x}) \in \mathbb{R}^r$ .

#### **Example (Square root graphical model)**

Let 
$$p(\mathbf{x} \mid \boldsymbol{\theta}) \propto \exp\left(-\sqrt{\mathbf{x}}^T \boldsymbol{\Theta} \sqrt{\mathbf{x}}\right), \ \mathbf{x} \in \mathbb{R}_+^m$$
. Then,

$$\Gamma(\mathbf{x}) = \operatorname{diag}(1/\mathbf{x}) \otimes \sqrt{\mathbf{x}} \sqrt{\mathbf{x}}^T \in \mathbb{R}^{m^2 \times m^2}$$

### **Robust score matching - considerations**



Standard score matching estimator  $\hat{\boldsymbol{\theta}} := \operatorname{argmin}_{\boldsymbol{\theta}} \ \frac{1}{2} \boldsymbol{\theta}^T \, \bar{\boldsymbol{\Gamma}} \, \boldsymbol{\theta} + \boldsymbol{\theta}^T \bar{\mathbf{g}} \text{ with } \bar{\boldsymbol{\Gamma}} := \frac{1}{n} \sum_{i=1}^n \boldsymbol{\Gamma}(\mathbf{x}_i).$  Estimator not robust, e.g. against  $\|\boldsymbol{\Gamma}(\mathbf{x}_1)\| \to \infty$ .

Desiderata for alternatives  $\hat{\Gamma}, \hat{g}$ 

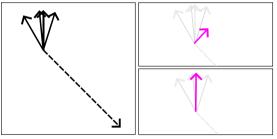
- Robust against arbitrary contamination of a few observations  $\mathbf{x}_i$  (i.e. rowwise contamination)
- Few assumptions on  $\Gamma, g$  required
- Computable in high dimensions
- $\hat{\Gamma}$  should be positive (semi)definite

#### The geometric median



Definition: Med $(\mathbf{x}_1, \dots, \mathbf{x}_n) := \operatorname{argmin}_{\mathbf{m}} \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{m}\|_2$ 

Illustration:



Mean

Geometric median

- Robustness and computation well studied in the literature
- Geometric median exists & unique under mild assumptions
- lacksquare  $\operatorname{Med}(\mathbf{x}_1,\ldots,\mathbf{x}_n) \in \mathsf{ConvHull}(\mathbf{x}_1,\ldots,\mathbf{x}_n)$ 
  - $\Rightarrow$  When  $\Gamma(\mathbf{x}_i)$  is pos. sem. def., then so is  $\operatorname{Med}(\Gamma(\mathbf{x}_1),\ldots,\Gamma(\mathbf{x}_n))$

### **Robust Score Matching**



We consider 
$$\hat{\boldsymbol{\theta}} := \operatorname{argmin}_{\boldsymbol{\theta}} \ \frac{1}{2} \boldsymbol{\theta}^T \hat{\boldsymbol{\Gamma}} \, \boldsymbol{\theta} + \boldsymbol{\theta}^T \hat{\mathbf{g}}$$
 with  $\hat{\boldsymbol{\Gamma}} := \operatorname{Med}(\boldsymbol{\Gamma}(\mathbf{x}_1), \dots, \boldsymbol{\Gamma}(\mathbf{x}_n))$ .

Additionally, we allow for

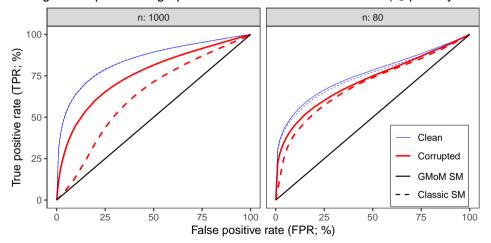
- lacksquare  $\ell_1$ -regularization
- support constraints (e.g. x > 0; generalized score matching)
- median-of-means to balance bias with robustness.

For pairwise interaction models, we prove edge recovery under standard Lasso-assumptions, even if a fraction of the n observations is arbitrarily contaminated.

### Simulation results for graphical models



Task: find edges in square root graphical model. Below: ROC curves ( $\ell_1$ -penalty varies)



#### **Outline**



- Score Matching using the Geometric Median (AISTATS 2025)
- Some phenomena in high dimensions (arXiv:2508.12926)

### Bias in high dimensions



Observation from robust score matching:

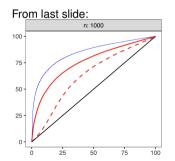
On uncorrupted data, geometric median-based  $\hat{\Gamma}$  surprisingly close to sample mean  $\bar{\Gamma}$  when

- $\blacksquare$  sample size n is large and
- number of observed variables is high.

Large-n-limit: Given random variable  $\mathbf{x} \in \mathbb{R}^p$ , define

- $\mathbf{m} := \operatorname{Med}(\mathbf{x}) := \operatorname{argmin}_{\tilde{\mathbf{m}}} \operatorname{E}[\|\mathbf{x} \tilde{\mathbf{m}}\|]$
- $\mu := E[x].$

Research Question: Quantify  $\|\mathbf{m} - \boldsymbol{\mu}\|$  as  $p \to \infty$ .





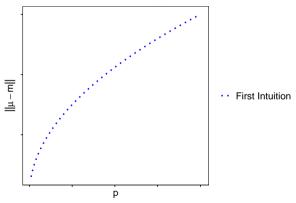
Consider  $\mathbf{x} \in \mathbb{R}^p$  with  $x_i$  iid. Exp(1). Geometric median  $\mathbf{m}$  exists & unique. How does  $\|\mathbf{m} - \boldsymbol{\mu}\|$  scale with p?



Consider  $\mathbf{x} \in \mathbb{R}^p$  with  $x_i$  iid. Exp(1). Geometric median  $\mathbf{m}$  exists & unique.

How does  $\|\mathbf{m} - \boldsymbol{\mu}\|$  scale with p?

First intuition: Componentwise median  $\tilde{\mathbf{m}}$  has  $\|\tilde{\mathbf{m}} - \boldsymbol{\mu}\| = |\log(2) - 1| \cdot \sqrt{p}$ 

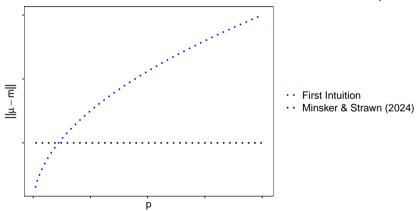




Consider  $\mathbf{x} \in \mathbb{R}^p$  with  $x_i$  iid. Exp(1). Geometric median  $\mathbf{m}$  exists & unique.

How does  $\|\mathbf{m} - \boldsymbol{\mu}\|$  scale with p?

First intuition: Componentwise median  $\tilde{\mathbf{m}}$  has  $\|\tilde{\mathbf{m}} - \boldsymbol{\mu}\| = |\log(2) - 1| \cdot \sqrt{p}$ 

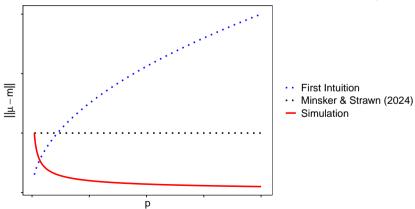




Consider  $\mathbf{x} \in \mathbb{R}^p$  with  $x_i$  iid. Exp(1). Geometric median  $\mathbf{m}$  exists & unique.

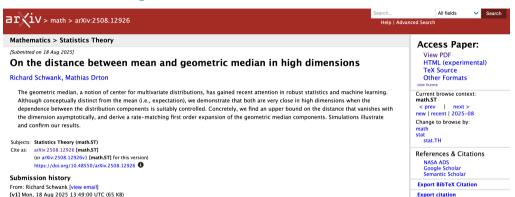
How does  $\|\mathbf{m} - \boldsymbol{\mu}\|$  scale with p?

First intuition: Componentwise median  $\tilde{\mathbf{m}}$  has  $\|\tilde{\mathbf{m}} - \boldsymbol{\mu}\| = |\log(2) - 1| \cdot \sqrt{p}$ 



#### **Theoretical insights**





We prove  $\| \boldsymbol{\mu} - \mathbf{m} \| = \mathcal{O} \left( \frac{1}{\sqrt{p}} \right)$  when components are M-dependent.

## **Discussion & Implications**



- Similarities with (Brown 1983): sample geometric median becomes efficient for isotropic Gaussian as  $p \to \infty$
- If M-dependence  $\approx$  edge sparsity, can explain Robust SM's small bias on uncorrupted data
- lacktriangle Consistency check: rowwise contaminated observations generally *not* M-dependent
- Note: certain *cellwise* contaminated observations are *M*-dependent. Indeed, geometric median *not* robust (Raymaekers and Rousseeuw 2024)
- "Robustness" depends on contamination assumption!

### Thank you!



- Schwank, R., McCormack, A., Drton, M. (2025). Robust score matching, AISTATS 2025.
- Schwank, R., Drton, M. (2025). On the distance between mean and geometric median in high dimensions. 10.48550/arXiv.2508.12926.

Contact: richard.schwank@tum.de

With funding from the:

Federal Ministry
of Research, Technology
and Space







This work is supported by the DAAD programme Konrad Zuse Schools of Excellence in Artificial Intelligence, sponsored by the Federal Ministry of Research, Technology and Space.

#### References



- Brown, B. M. (Sept. 1983). "Statistical Uses of the Spatial Median". In: Journal of the Royal Statistical Society: Series B (Methodological) 45.1, pp. 25–30. ISSN: 2517-6161. DOI: 10.1111/j.2517-6161.1983.tb01226.x.
- Minsker, Stanislav and Nate Strawn (July 2023). "The Geometric Median and Applications to Robust Mean Estimation". In: DOI: 10.48550/ARXIV.2307.03111. arXiv: 2307.03111 [math.ST].
- Raymaekers, Jakob and Peter J. Rousseeuw (Feb. 2024). "Challenges of cellwise outliers". In: *Econometrics and Statistics*. ISSN: 2452-3062. DOI: 10.1016/j.ecosta.2024.02.002.