# Fat-Tailed Variational Inference with Anisotropic Tail Adaptive Flows

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### Variational inference

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**Variational inference**:  $\max_{q \in \mathcal{Q}} \mathtt{ELBO}(q, \bar{\pi})$  where

$$- ext{KL}(q,\pi) \propto ext{ELBO}(q,ar{\pi}) = \int q(x) \log rac{ar{\pi}(x)}{q(x)} dx \ pprox rac{1}{n} \sum_{i=1}^n \log rac{ar{\pi}(x_i)}{q(x_i)}, \; x_i \stackrel{ ext{i.i.d.}}{\sim} q$$

More expressive variational family  $\mathcal{Q}\Rightarrow$  better approximation quality



# Expressive variational families using flows

Let  $f_{\theta}$  be an invertible flow and  $p_X(x)$  a probability density (the *base distribution*). Consider variational family  $\mathcal{Q} = \{q_{\theta} : \theta \in \Theta\}$  where

$$q_{\theta}(y) = \rho_{X}(f_{\theta}^{-1}(y)) \left| \det \frac{df_{\theta}^{-1}(z)}{dz} \right|_{z=y}. \tag{1}$$

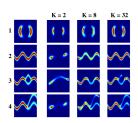


Figure 1: From [15], flows can transform a Gaussian into complex pushforward distributions



Model	Autoregressive transform	Lipschitz when
NICE[3]	$z_j + \mu_j \cdot \mathbb{1}_{k  ot \in [j]}$	$\mu_j$ Lipschitz
MAF[14]	$\sigma_j z_j + (1 - \sigma_j) \mu_j$	$\sigma_j$ bounded
IAF[12]	$z_j \cdot \exp(\lambda_j) + \mu_j$	$\lambda_j$ bounded, $\mu_j$ Lipschitz
Real-NVP[4]	$\exp(\lambda_j \cdot \mathbb{1}_{k \notin [j]}) \cdot z_j + \mu_j \cdot \mathbb{1}_{k \notin [j]}$	$\lambda_j$ bounded, $\mu_j$ Lipschitz
Glow[11]	$\sigma_j \cdot z_j + \mu_j \cdot \mathbb{1}_{k \not\in [j]}$	$\sigma_j$ bounded, $\mu_j$ Lipschitz
NAF[8]	$\sigma^{-1}(\mathbf{w}^{\top}\cdot\sigma(\sigma_{j}\mathbf{z}_{j}+\mu_{j}))$	Always (logistic mixture CDF)
NSF[5]	$z_{j} \mathbb{1}_{z_{j} \notin [-B,B]} + M_{j}(z_{j}; z_{< j}) \mathbb{1}_{x_{j} \in [-B,B]}$	Always (linear outside $[-B,B]$ )
FFJORD[7]	n/a (not autoregressive)	Always (required for invertibility)
ResFlow[2]	n/a (not autoregressive)	Always (required for invertibility)

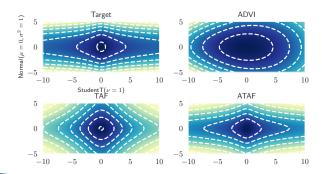
Table 1: Some recently developed invertible flows.



#### Fat-tailed variational inference

#### **Our Research Aims:**

- What happens when  $\pi$  is fat-tailed?
- What about when  $\pi$  is multivariate?





### Methods

#### Automatic Differentiation Variational Inference (ADVI, [13, 17]):

$$Q_{\text{ADVI}} := \{(f_{\theta})_* \mu\}, \text{ where } \mu = \text{Normal}(0_d, I_d).$$

#### Tail Adaptive Flows (TAF, [9]):

$$\mathcal{Q}_{\mathsf{TAF}} \coloneqq \{(f_{\theta})_* \mu_{\nu}\}$$
, where  $\mu_{\nu} = \prod_{i=1}^d \mathsf{StudentT}(\nu)$  with  $\nu \in \mathbb{R}_+$ .

#### Anisotropic Tail-Adaptive Flows (ATAF, this work):

$$\mathcal{Q}_{\mathsf{ATAF}} \ := \ \{(f_{\theta})_*\mu_{oldsymbol{
u}}\}, \, \mathsf{where} \, \mu_{oldsymbol{
u}} = \prod_{i=1}^d \mathsf{StudentT}(
u_i) \, \mathsf{with} \, oldsymbol{
u} \in \mathbb{R}^d_+.$$



# Sharpening prior univariate theory

### Assumption

 $f_{\theta}$  is invertible, and both  $f_{\theta}$  and  $f_{\theta}^{-1}$  are L-Lipschitz continuous (e.g. Table 1).

#### Theorem

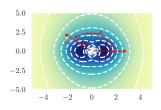
- $f_{\theta}$  cannot make the tails of a fat-tailed distribution fatter (decrease tail parameter  $\alpha$ ).
- If in addition  $f_{\theta}$  is smooth with no critical points, then it cannot change the tail parameter of a fat-tailed distribution.
- Light-tailed distributions remain light-tailed under polynomial flows [10].

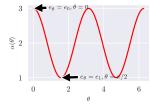


# Multivariate fat tails and tail anisotropy

#### Definition (Tail parameter function)

For random vector X, define  $\alpha_X(v) = -\lim_{x \to \infty} \log \mathbb{P}(\langle v, X \rangle \geq x)/\log x$  when the limit exists, and  $\alpha_X(v) = +\infty$  otherwise. X is *tail-isotropic* if  $\alpha_X(v) \equiv c < \infty$  is constant.







## **Necessity of ATAF**

### Proposition (Pushforwards of tail-isotropic distributions)

Let  $\mu$  be tail isotropic with non-integer parameter  $\nu$  and suppose  $f_{\theta}$  satisfies Assumption 1. Then  $(f_{\theta})_*\mu$  is tail isotropic with parameter  $\nu$ .



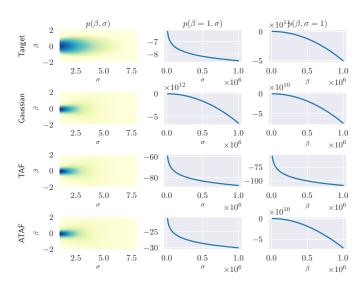
# Bayesian linear regression

$$\sigma^2 \sim \mathsf{Inv ext{-}Gamma}(a_0,b_0)$$
  $eta \mid \sigma^2 \sim \mathcal{N}(0,\sigma^2), \qquad \mathsf{v} \mid \mathsf{X}, eta, \sigma \sim \mathcal{N}(\mathsf{X}eta,\sigma^2),$ 

The posterior is tail-anisotropic:

$$\begin{split} &\rho(\sigma^2,\beta=c\mid \textbf{X},\textbf{y}) \propto \rho(\sigma^2) \in \mathcal{L}^1_{\alpha_n} \text{ is fat-tailed (power-law)} \\ &\rho(\sigma^2=c,\beta\mid \textbf{X},\textbf{y}) \propto \rho(\beta\mid c) \in \overline{\mathcal{E}^2} \text{ is light-tailed (sub-Gaussian)} \end{split}$$







# Eight schools [16]

$$\begin{split} \tau \sim \text{HalfCauchy(loc} &= 0, \text{scale} = 5) \\ \mu \sim \mathcal{N}(0, 5), & \theta \sim \mathcal{N}(\mu, \tau), & \text{y} \sim \mathcal{N}(\theta, \sigma). \end{split}$$

	ELBO	$\log p(y)$
ADVI	$-72.13 \pm 6.89$	$-53.25 \pm 3.44$
TAF	$-64.64 \pm 4.88$	$-52.51 \pm 4.41$
ATAF	$-58.63 \pm 4.75$	$-51.01 \pm 3.71$
NUTS	n/a	$-47.78 \pm 0.093$



# Financial [6] and actuarial [1] density modeling

	Fama-French 5 Industry Daily	CMS 2008-2010 DE-SynPUF
ADVI	$-5.018 \pm 0.056$	$-1.883 \pm 0.012$
TAF	$-4.703 \pm 0.023$	$-1.659 \pm 0.004$
ATAF	$-4.699 \pm 0.024$	$-1.603 \pm 0.034$

Table 2: Log-likelihoods (higher is better,  $\pm$  standard errors).



### Conclusions

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- Flow-based VI can expressively model the bulks of complicated distributions ...
- But modeling of tails is still limited by choice of base distribution!
- We improved prior work (TAF, [9]), which considered univariate tails, to do:
  - $\,$  Prior univariate theory is refined to include  $\alpha$  and closure results are sharpened
  - A multivariate theory is proposed to quantify tail-anisotropy and prove ATAF's necessity
  - Experiments confirm ATAF's improvements on real-world fat-tailed datasets



#### References I

- [1] Centers for Medicare and Medicaid Services. CMS 2008-2010 data entrepreneurs' synthetic public use file (DE-SynPUF), 2010. [Online; accessed 10-March-2020].
- [2] Ricky TQ Chen, Jens Behrmann, David K Duvenaud, and Jörn-Henrik Jacobsen. Residual flows for invertible generative modeling. Advances in Neural Information Processing Systems, 32:9913–9923, 2019.
- [3] L Dinh, D Krueger, and Y Bengio. NICE: non-linear independent components estimation. In *3rd International Conference on Learning Representations, Workshop Track Proceedings*, 2015.
- [4] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real NVP. In *5th International Conference on Learning Representations*, 2017.
- [5] Conor Durkan, Artur Bekasov, Iain Murray, and George Papamakarios. Neural spline flows. Advances in Neural Information Processing Systems, 32:7509–7520, 2019.



#### References II

- [6] Eugene F Fama and Kenneth R French. A five-factor asset pricing model. *Journal of Financial Economics*, 116(1):1–22, 2015.
- [7] Will Grathwohl, Ricky T. Q. Chen, Jesse Bettencourt, Ilya Sutskever, and David Duvenaud. FFJORD: free-form continuous dynamics for scalable reversible generative models. In *International Conference on Learning Representations*, 2019.
- [8] Chin-Wei Huang, David Krueger, Alexandre Lacoste, and Aaron Courville. Neural autoregressive flows. In *International Conference on Machine Learning*, pages 2078–2087. PMLR, 2018.
- [9] Priyank Jaini, Ivan Kobyzev, Yaoliang Yu, and Marcus Brubaker. Tails of Lipschitz triangular flows. In *International Conference on Machine Learning*, pages 4673–4681. PMLR, 2020.
- [10] Priyank Jaini, Kira A Selby, and Yaoliang Yu. Sum-of-squares polynomial flow. In *International Conference on Machine Learning*, pages 3009–3018. PMLR, 2019.



#### References III

- [11] Diederik P. Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. *Advances in Neural Information Processing Systems*, 31:10236–10245, 2018.
- [12] Diederik P. Kingma, Tim Salimans, Rafal Józefowicz, Xi Chen, Ilya Sutskever, and Max Welling. Improving variational autoencoders with inverse autoregressive flow. Advances in Neural Information Processing Systems, 29:4736–4744, 2016.
- [13] Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David M Blei. Automatic differentiation variational inference. *The Journal of Machine Learning Research*, 18(1):430–474, 2017.
- [14] George Papamakarios, Theo Pavlakou, and Iain Murray. Masked autoregressive flow for density estimation. *Advances in Neural Information Processing Systems*, 30:2338–2347, 2017.



#### References IV

- [15] Danilo Rezende and Shakir Mohamed. Variational inference with normalizing flows. In *International Conference on Machine Learning*, pages 1530–1538. PMLR, 2015.
- [16] Donald B Rubin. Estimation in parallel randomized experiments. *Journal of Educational Statistics*, 6(4):377–401, 1981.
- [17] Stefan Webb, J.P. Chen, Martin Jankowiak, and Noah Goodman. Improving automated variational inference with normalizing flows. *6th ICML Workshop on Automated Machine Learning (AutoML)*, 2019.

