Conditional Sampling with Monotone GANs

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Problem Setting

Setting

Target measure: $\nu(dx, dy)$ supported on $\mathbb{R}^{n+m}$

Data: $\{x_n, y_n\}_{n=1}^{N} \overset{i.i.d.}{\sim} \nu.$

Goal: sample $\nu(dy|x)$ for any $x \in \operatorname{supp} \nu(dx)$

Approach

Reference measure : $\eta(dy)$ supported on $\mathbb{R}^m$

Approximate: $S(x, \cdot) : \mathbb{R}^m \to \mathbb{R}^m$ s.t.

$$S(x, \cdot)_\sharp \eta(dy) = \nu(dy|x)$$

Key Idea

Construct block-triangular $T : \mathbb{R}^{n+m} \to \mathbb{R}^{n+m}$ s.t. $T_\sharp \eta(dx, dy) = \nu$ and extract S.

Applications

Probabilistic Supervised Learning and UQ

Model: $y = G(x)$, with G stochastic mapping

Statsitics of $y|x$: mean, median, maximal probability points, variance, confidence intervals, error bars, etc.

Does not require knowledge of G, only data.

Bayesian Inverse Problem

Model: $x = G(y)$, with G stochastic mapping

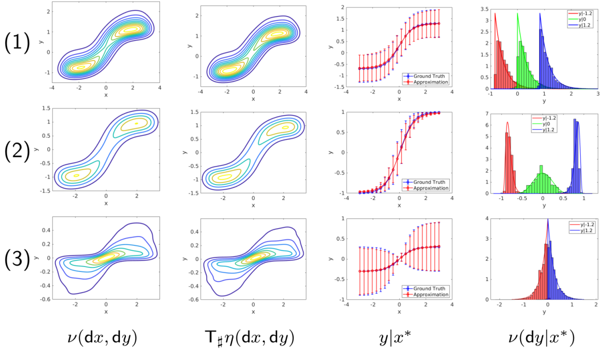
Characterize posterior $y|x$.

Does not require a know prior on parameters, only data.

1D Example

Different noise models

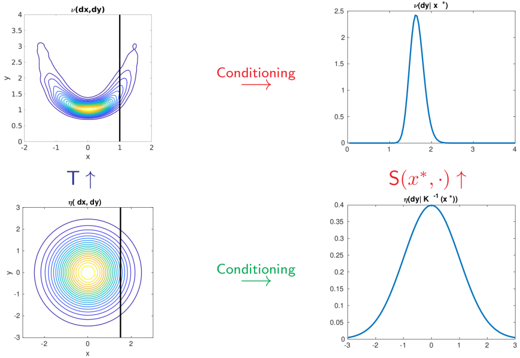
$$y = \tanh(x) + \gamma, \qquad \gamma \sim \Gamma(1, 0.3) \qquad (1)$$
$$y = \tanh(x + \gamma), \qquad \gamma \sim N(0, 0.05) \qquad (2)$$
$$y = \gamma \tanh(x), \qquad \gamma \sim \Gamma(1, 0.3) \qquad (3)$$



Block-triangular map

$$\text{Joint: } T(x,y) = \begin{bmatrix} K(x) \\ S(K(x),y) \end{bmatrix}, \quad K : \mathbb{R}^n \to \mathbb{R}^n, S : \mathbb{R}^{n+m} \to \mathbb{R}^m$$

$$\text{Conditioning: } S(x,y)$$



Block-triangular measure transport

Properties

- Block-triangular mappings exist under mild conditions (e.g. ν and η are absolutely continuous without atoms).
- Block-triangular maps can be constructed explicitly (e.g. the Knothe-Rosenblatt rearrangement).

Optimization

$$\begin{aligned}
\text{Objective:}\quad & T = \operatorname*{arg\,min}_{T \in \mathcal{T}} D(T_\sharp \eta(dx, dy) || \nu(dx, dy)) \\
\text{Statistical Divergence:}\quad & D : \mathcal{P}(\mathbb{R}^{n+m}) \times \mathcal{P}(\mathbb{R}^{n+m}) \to \mathbb{R}_+ \\
& \text{s.t. } D(\mu, \nu) = 0 \text{ iff } \mu = \nu \\
\text{Approximation Space:}\quad & \mathcal{T} = \{\text{block-triangular, continuous, monotone maps}\}
\end{aligned}$$

Block-triangular measure transport

$$T^* = \arg\min_{T \in \mathcal{T}} D(T_\sharp \eta(dx, dy) || \nu(dx, dy)) \qquad (1)$$

Theorem [KBHM 20]

Let T^* be given by (1) and suppose it has the form

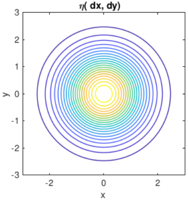
$$T^*(x, y) = \begin{bmatrix} K^*(x) \\ S^*(K^*(x), y) \end{bmatrix}.$$

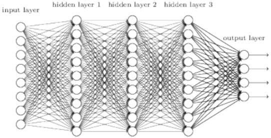
If T^* is surjective then for any $x \in \operatorname{supp} \nu(dx)$, we have that

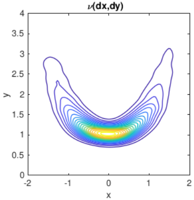
$$S^*(x, \cdot)_\sharp \eta(dy) = \nu(dy|x).$$

- By Browder-Minty theorem: continuity + monotonicity + coercivity $\implies$ surjectivity.

GANs


η(dx, dy)
3
2
1
0
-1
-2
-3
-2
0
2
x
y


input layer
hidden layer 1
hidden layer 2
hidden layer 3
output layer


ν(dx,dy)
4
3.5
3
2.5
2
1.5
1
0.5
0
-2
-1
0
1
2
x
y

The GAN "divergence"

Objective: $T^* = \arg\min_{T \in \mathcal{T}} D_{\text{GAN}}(T_\sharp \eta || \nu)$

Divergence: $D_{\text{GAN}}(T_\sharp \eta || \nu) = \sup_{f \in C(\mathbb{R}^{n+m};[0,1])} \mathbb{E}_{z \sim \nu} \log f(z) + \mathbb{E}_{w \sim \eta} \log(1 - f(T(w)))$

Approximation Space

Choose $\mathcal{T}$ as the set of continuous, strictly monotone, block-triangular mappings:

$$\begin{cases} T(x,y) = \begin{bmatrix} K(x) \\ S(K(x),y) \end{bmatrix} \in C(\mathbb{R}^{n+m};\mathbb{R}^{n+m}) \\ \langle T(w) - T(w'), w - w' \rangle > 0, \quad \eta - \text{a.e.} \end{cases}$$

Discretize

Data: $\{z_j = (x_j, y_j)\}_{j=1}^N \overset{i.i.d.}{\sim} \nu$

Reference samples: $\{w_k\}_{k=1}^{2J} \overset{i.i.d.}{\sim} \eta$

Neural Networks: K, S, f

Divergence: $$\min_f \frac{1}{N}\sum_{j=1}^N \log f(z_j) + \frac{1}{2J}\sum_{k=1}^{2J} \log(1 - f(T(w_k)))$$

Average Monotonicity: $$\frac{1}{J}\sum_{k=1}^{J} \langle T(w_k) - T(w_{k+J}), w_k - w_{k+J} \rangle > 0$$

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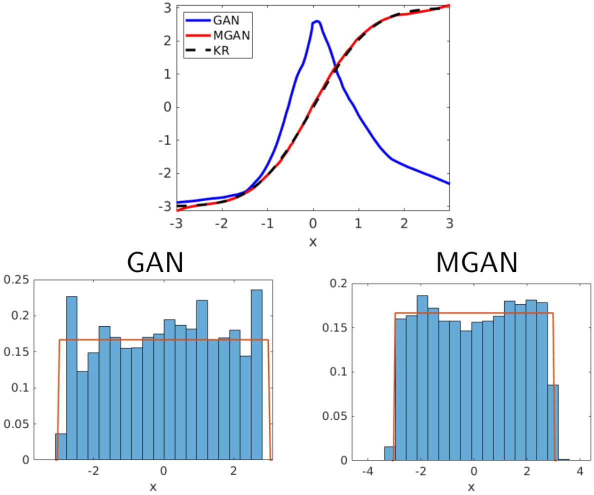
GANs: Monotonicity

- $\nu = U(-3,3)$, $\eta = N(0,1)$



GANs: Sampling and UQ

$$T^* = \arg\min_{T \in \mathcal{T}} D_{\mathrm{GAN}}(T_\sharp \eta || \nu)$$

- Extract $S^*(x, y)$ from $T^*(x, y)$.
- New input $x^\dagger \in \mathbb{R}^n$.
- Generate new samples from reference marginal $\tilde{y}_k \overset{i.i.d.}{\sim} \eta(dy)$.
- Set $y_k = S(x^\dagger, \tilde{y}_k)$ then $y_k \sim \nu(dy|x^\dagger)$.
- Use y_k to compute statistics of $\nu(dy|x^\dagger)$.

Example: Blood Oxygen Demand Model

Model

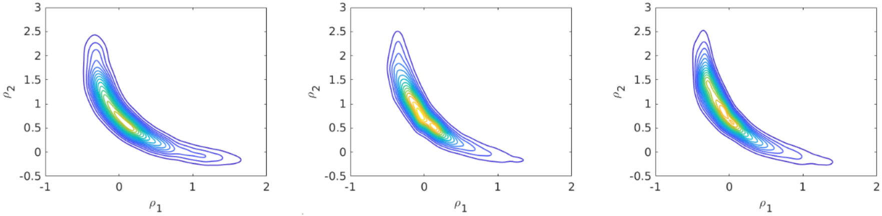
$$\begin{aligned} \text{Model:} \quad & B(t) = A(1 - e^{-Bt}) + \gamma \\ \text{Prior:} \quad & A \sim U(0.4, 1, 2), B \sim U(0.01, 0.31) \\ \text{Noise:} \quad & \gamma \sim N(0, 10^{-3}) \end{aligned}$$

Data

$$\begin{aligned} \text{Without prior:} \quad & x = (B(1), B(2), \dots, B(5)), y = (A, B) \\ \text{With prior:} \quad & x = (B(1), B(2), \dots, B(5)), \\ & y = \left(\rho_1 = \sqrt{2}\mathrm{erf}^{-1}\left(\frac{A - 0.4}{0.4} - 1\right), \rho_2 = \sqrt{2}\mathrm{erf}^{-1}\left(\frac{A - 0.01}{0.15} - 1\right)\right) \\ & \text{s.t. } (\rho_1, \rho_2) \sim N(0, I_2) \end{aligned}$$

Example: Blood Oxygen Demand Model

Map type	N	Mean		Variance		Skewness		Kurtosis	
		ρ_1	ρ_2	ρ_1	ρ_2	ρ_1	ρ_2	ρ_1	ρ_2
MCMC "truth"		0.075	0.875	0.190	0.397	1.935	0.681	8.537	3.437
[30]	5000	0.090	**0.908**	0.180	0.490	2.968	**0.707**	29.589	16.303
	50000	0.034	0.902	0.206	0.457	1.628	0.872	7.568	3.876
MGAN (without prior)	5000	**0.075**	0.762	**0.193**	0.331	1.079	0.451	3.980	**3.048**
	50000	**0.071**	0.843	**0.196**	0.358	**2.003**	**0.538**	7.961	3.246
MGAN (with prior)	5000	0.084	0.805	0.278	**0.402**	**1.947**	0.805	**8.122**	4.363
	50000	0.038	**0.882**	0.205	**0.397**	2.132	0.490	**8.9747**	**3.408**



(a) MCMC (b) Without prior (c) With prior

Example: Darcy Flow

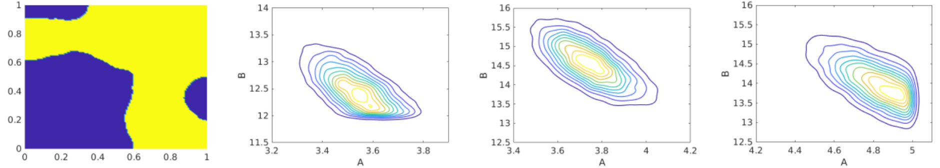
Model

$$\begin{aligned} \text{Model:} \quad & -\nabla \cdot (a \nabla p) = f \\ & a(s) = A\mathbb{1}_{\Omega_A} + B\mathbb{1}_{\Omega_B} \\ \text{Prior:} \quad & A \sim U(3,5), B \sim U(12,16) \\ \text{Noise (additive):} \quad & \gamma \sim N(0, 10^{-7} I_{16}) \end{aligned}$$

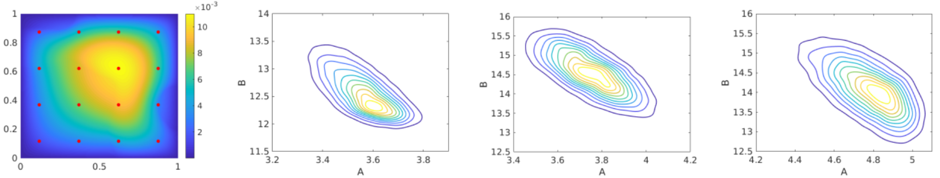
Data

$$\text{Without prior:} \quad x = (p(1), p(2), \ldots, p(16)), y = (A, B)$$

Example: Darcy Flow



(a) Ω_A, Ω_B (b) MCMC $\boldsymbol{y}|\boldsymbol{x}_1^*$ (c) MCMC $\boldsymbol{y}|\boldsymbol{x}_2^*$ (d) MCMC $\boldsymbol{y}|\boldsymbol{x}_3^*$



(e) $\boldsymbol{x}_2^*$ (f) $\mathsf{F}_\sharp(\boldsymbol{x}_1^*, \cdot)\eta(\boldsymbol{y})$ (g) $\mathsf{F}_\sharp(\boldsymbol{x}_2^*, \cdot)\eta(\boldsymbol{y})$ (h) $\mathsf{F}_\sharp(\boldsymbol{x}_3^*, \cdot)\eta(\boldsymbol{y})$

Example: MNIST

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Conditional Sampling

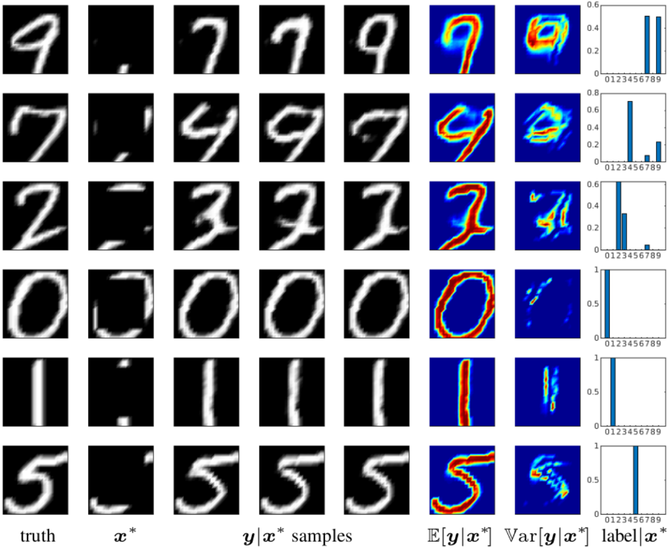
N.B.K.

Problem Setting

Block-triangular measure transport

GANs

Numerics



Conclusion

- A model agnostic method for probabilistic supervised learning.
- Applications to Bayesian inverse problems.
- Using measure transport for conditioning.
- A straightforward extension of GAN framework.
- Future extensions:
  - Generalize to infinite dimensions.
  - Analysis: approximations of T and the pushforward $T_\sharp \eta$, properties of the minimizer, sample sizes, choice of divergence, etc.