MParT: Monotone Parameterization Toolkit

Scaling Measure Transport for High-dimensional Conditional Inference Problems

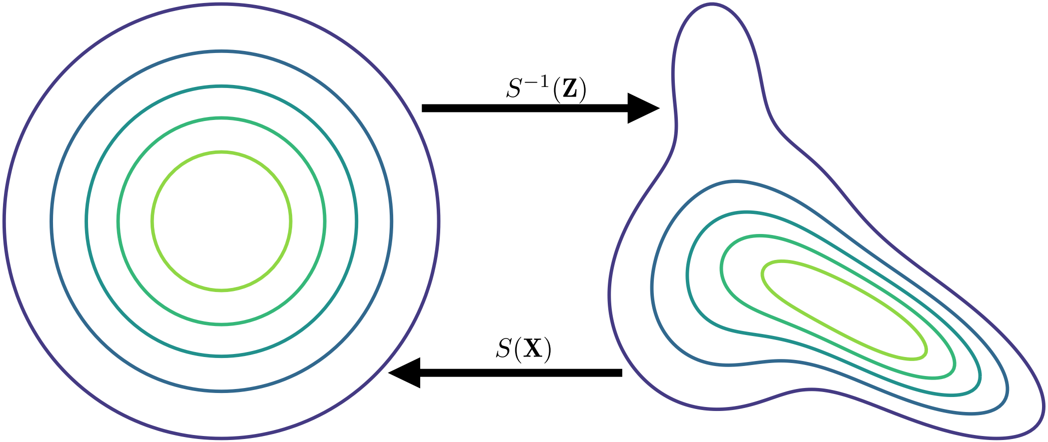
Daniel Sharp[1] **Matthew Parno**[2] **Michael Brennan**[1] **Youssef Marzouk**[1]

[1]Massachusetts Institute of Technology

[2]Solea Energy

February 28, 2024

Measure Transport



Why solve this?

- Variational Inference
- Generative Modeling
- Density Estimation
- Data Assimilation
- **Conditional Sampling/Simulation-based Inference**

Why solve this?

- Variational Inference
- Generative Modeling
- Density Estimation
- Data Assimilation
- Conditional Sampling/Simulation-based Inference

Why solve this?

- Variational Inference
- Generative Modeling
- Density Estimation
- Data Assimilation
- **Conditional Sampling/Simulation-based Inference**

$$\pi_{X|Y} \propto \pi_{Y|X}\pi_X$$

Problem to Solve

$$S_j(\mathbf{x}) \text{ s.t. } \frac{\partial}{\partial x_n} S_j(\mathbf{x}_{1:n-1}, x_n) > 0$$

$$S(\mathbf{x}) = \begin{bmatrix} S_1(x_1) \\ S_2(x_1, x_2) \\ \vdots \\ S_n(\mathbf{x}_{1:n-1}, x_n) \end{bmatrix}$$

$$\nabla S(\mathbf{x}) = \begin{bmatrix} \partial_1 S_1 & 0 & \cdots & 0 \\ \partial_1 S_2 & \partial_2 S_2 & & 0 \\ \vdots & & \ddots & \vdots \\ \partial_1 S_n & \partial_2 S_n & \cdots & \partial_n S_n \end{bmatrix}$$

Why triangular? (Computational)

$$S_1(X_1) = Z_1^* \qquad X_1 = S_1(\cdot)^{-1}\left(Z_1^*\right)$$

$$S_2(X_1, X_2) = Z_2^* \qquad X_2 = S_2(X_1, \cdot)^{-1}\left(Z_2^*\right)$$

$$S_3(X_1, X_2, X_3) = Z_3^* \qquad X_3 = S_3(X_1, X_2, \cdot)^{-1}\left(Z_3^*\right)$$

$$\vdots$$

Why triangular? (Computational)

$$S_1(X_1) = Z_1^* \qquad X_1 = S_1(\cdot)^{-1}(Z_1^*)$$

$$S_2(X_1, X_2) = Z_2^* \qquad X_2 = S_2(X_1, \cdot)^{-1}(Z_2^*)$$

$$S_3(X_1, X_2, X_3) = Z_3^* \qquad X_3 = S_3(X_1, X_2, \cdot)^{-1}(Z_3^*)$$

$$\vdots$$

Why triangular? (Computational)

$$S_1(X_1) = Z_1^* \qquad X_1 = S_1(\cdot)^{-1}\,(Z_1^*)$$

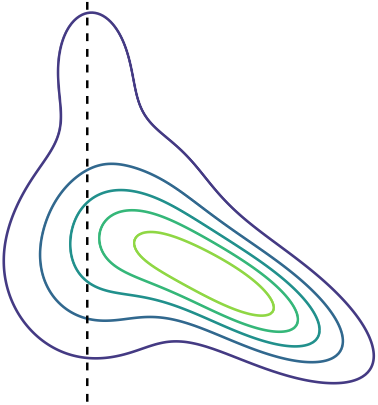
$$S_2(X_1, X_2) = Z_2^* \qquad X_2 = S_2(X_1, \cdot)^{-1}\,(Z_2^*)$$

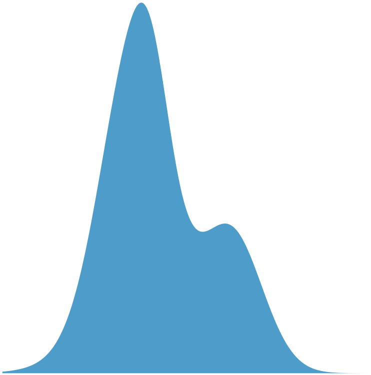
$$S_3(X_1, X_2, X_3) = Z_3^* \qquad X_3 = S_3(X_1, X_2, \cdot)^{-1}\,(Z_3^*)$$

$$\vdots$$

Why triangular? (Principle)

$$S(\mathbf{X}^*_{1:n-1}, X_n) = Z_n \qquad S(\mathbf{X}^*_{1:n-1}, \cdot)^{-1}(Z_n) = X_n \sim \pi_{X_n|\mathbf{X}^*_{1:n-1}}$$





What do we want?

- Finite training budget (i.e., "Training is not most expensive part")
- Fast evaluation and training for usage online or in loop-based inference
- Reliable, reproducible results
- Well-understood approximation theory

What do we want?

- Finite training budget (i.e., “Training is not most expensive part”)
- Fast evaluation and training for usage online or in loop-based inference
- Reliable, reproducible results
- Well-understood approximation theory

What MPart Brings (Software)

- **Fast, parallel, efficient Kokkos-based C++**
- **GPU support for map evaluation**
- **Easy installation with bindings to Python, Matlab, and Julia**
- PyTorch integration
- Out-of-the-box training with NLOpt
- Easy serialization
- Test-driven development, GitHub CI

```
$ pip install mpart
$ conda install conda-forge::mpart
julia> ]add MParT
$ cd build && cmake ..
```

What MParT Brings (Software)

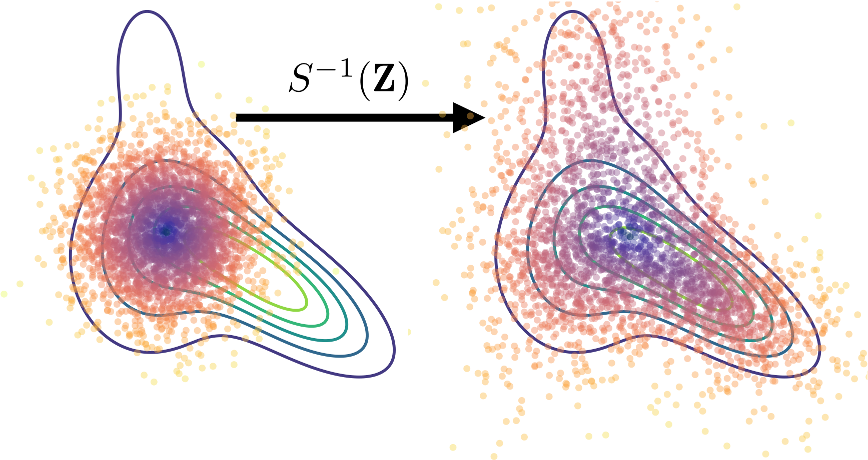
- **Fast, parallel, efficient Kokkos-based C++**
- **GPU support for map evaluation**
- **Easy installation with bindings to Python, Matlab, and Julia**
- PyTorch integration
- Out-of-the-box training with NLOpt
- Easy serialization
- Test-driven development, GitHub CI

```
$ pip install mpart
$ conda install conda-forge::mpart
julia> ]add MParT
$ cd build && cmake ..
```

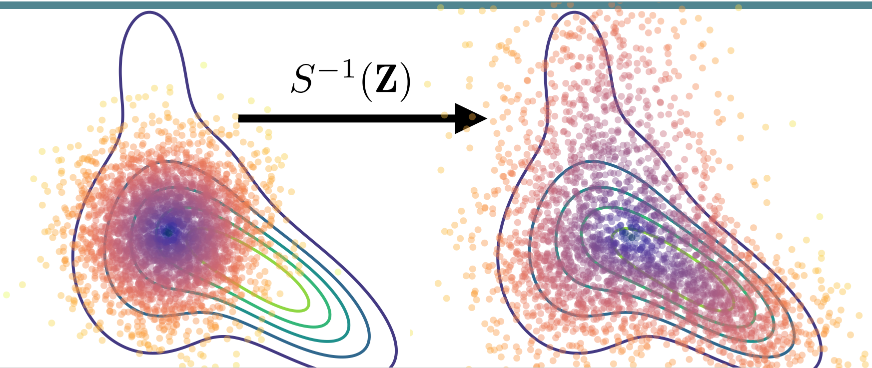
What MParT Brings (Approximation)

- Fast multivariate expansions and multi-index computation
- Specialized numerical quadrature and root-finding (on device)
- Evaluation, inversion, Jacobian-vector product, parameter gradients...
- Efficient map composition
- Adaptive multi-index set facilities

Small Example



Small Example




```
map_dim, totalOrder, basisType = 2, 4, "HermiteFunctions"
mapOpts = MapOptions(;basisType, basisLB=-4, basisUB=4)
trimap = CreateTriangular(map_dim, map_dim, totalOrder, mapOpts)
obj = CreateGaussianKLObjective(samples)
train_opts = TrainOptions()
TrainMap(trimap, obj, train_opts)
```

How to find S?

$$\mathcal{J}(S) = D_{KL}(\pi \| S^\sharp \rho)$$

$$\mathcal{J}_n(S_n) = \sum_{i=1}^{N} \left[\tfrac{1}{2} S_n(\mathbf{x}^{(i)})^2 - \log \partial_n S_n(\mathbf{x}^{(i)}) \right]$$

What gives us efficiency?

- Rectified integration

$$S_n(\mathbf{x}) = g(\mathbf{x}, 0) + \int_0^{x_n} r(\partial_n g(\mathbf{x}_{1:n-1}, t))\, dt, \quad g(\mathbf{x}) = \sum_{\vec{\alpha}} c_{\vec{\alpha}} \Psi_{\vec{\alpha}}(\mathbf{x}),\ r(x) > 0$$

- Rectified expansion (**NEW**)

$$S_n(\mathbf{x}) = g_1(\mathbf{x}_{1:n-1}) + \sum_{\vec{\beta}} r(\Psi_{\vec{\beta}}(\mathbf{x}_{1:n-1})) s_{\beta_n}(x_n), \qquad s'_{\beta_y}(x) > 0$$

What gives us efficiency?

- Rectified integration

$$S_n(\mathbf{x}) = g(\mathbf{x}, 0) + \int_0^{x_n} r(\partial_n g(\mathbf{x}_{1:n-1}, t))\; dt, \quad g(\mathbf{x}) = \sum_{\vec{\alpha}} c_{\vec{\alpha}} \Psi_{\vec{\alpha}}(\mathbf{x}),\; r(x) > 0$$

- Rectified expansion (**NEW**)

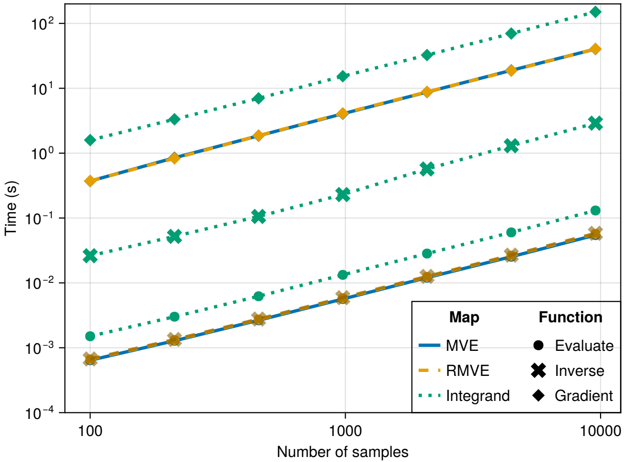
$$S_n(\mathbf{x}) = g_1(\mathbf{x}_{1:n-1}) + \sum_{\vec{\beta}} r(\Psi_{\vec{\beta}}(\mathbf{x}_{1:n-1})) s_{\beta_n}(x_n), \qquad s'_{\beta_y}(x) > 0$$

Scalability

- 1000 dimensions
- Max order 10
- Multi-indices:

$$g(\mathbf{x}) = \sum_{i,j=1}^{d,p} c_{ij}\psi_i(x_j)$$

- **10k parameters, 16 core CPU**



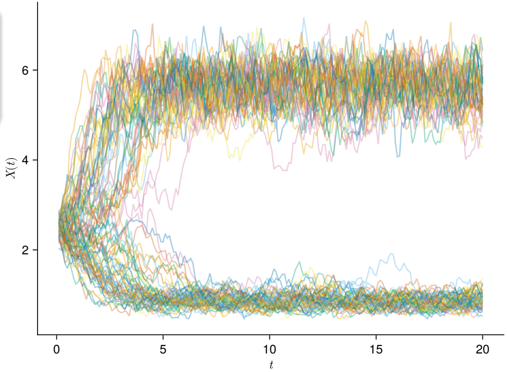
$$A + 2X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 3X$$

$$B \underset{k_4}{\overset{k_3}{\rightleftharpoons}} X$$

Sampling a stochastic process

Chemical reaction kinetics

[Sargsyan et al. 09]



Karhunen Loeve Expansion

$$u(t,\omega) = \mu(t) + \sum_{j=1}^{\infty} \sqrt{\lambda_j}\psi_j(t)X_j(\omega)$$

- ψ_j orthogonal
- X_j uncorrelated, mean 0, variance 1
- We can estimate μ, λ_j, ψ_j from samples
- We virtually never know how to sample X!

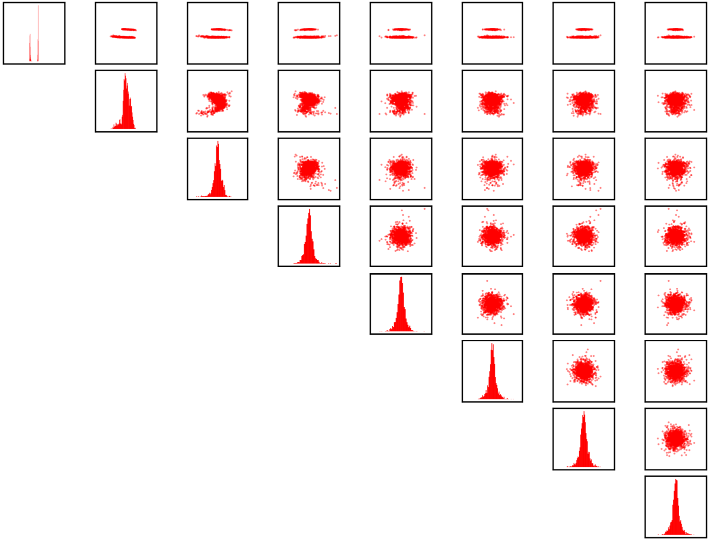
Karhunen Loeve Expansion

$$u(t,\omega) = \mu(t) + \sum_{j=1}^{\infty} \sqrt{\lambda_j}\psi_j(t)X_j(\omega)$$

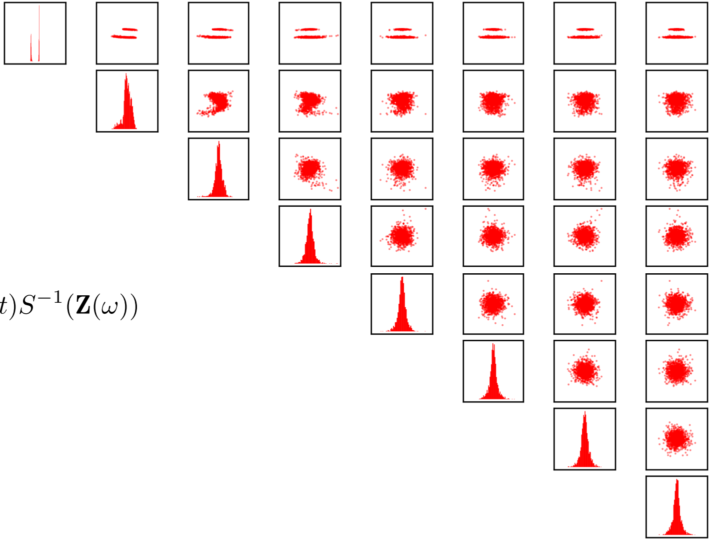
- ψ_j orthogonal
- X_j uncorrelated, mean 0, variance 1
- We can estimate μ, λ_j, ψ_j from samples
- **We virtually never know how to sample X!**

What if...

$$\sqrt{\lambda_j} X_j = \langle u - \mu, \psi_j \rangle$$



What if...

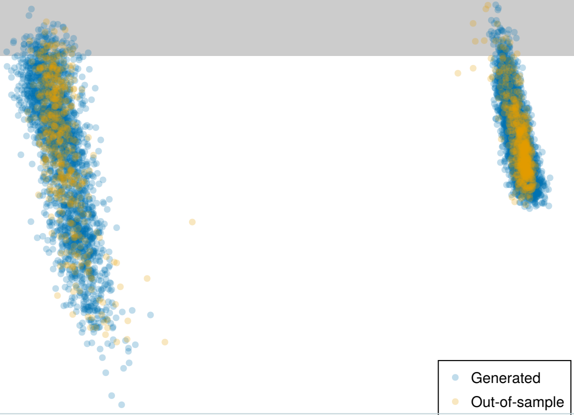


$$\sqrt{\lambda_j} X_j = \langle u - \mu, \psi_j \rangle$$

$$u(t,\omega) \approx \widehat{u}(t,\omega) = \mu(t) + \sum_{j=1}^{\infty} \psi_j(t) S^{-1}(\mathbf{Z}(\omega))$$

Results

```
minOrder, firstOrders=4, [15, 10]
multiindex_sets, opts = KLE_multi_index_setup(dim, minOrder, firstOrders)
map_components = [CreateComponent(mset, opts) for mset in multiindex_sets]
trimap = TriangularMap(map_components)
obj = CreateGaussianKLObjective(samples)
train_opts = TrainOptions()
TrainMap(trimap, obj, train_opts)
```

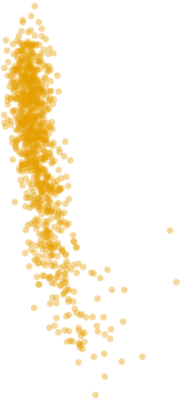


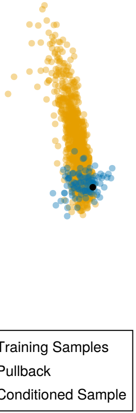
Conditional Sampling

$$S(u(t^*, \omega), X_1, \ldots)$$

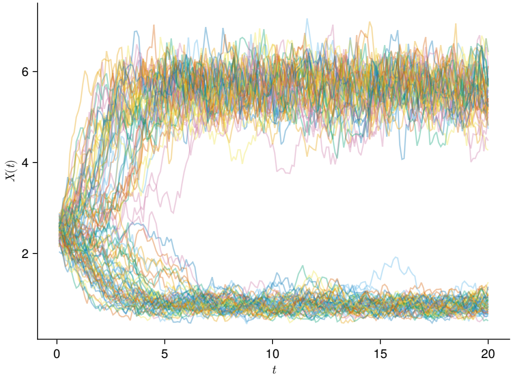
Conditional Sampling

$$S(u(t^*, \omega), X_1, \ldots)$$

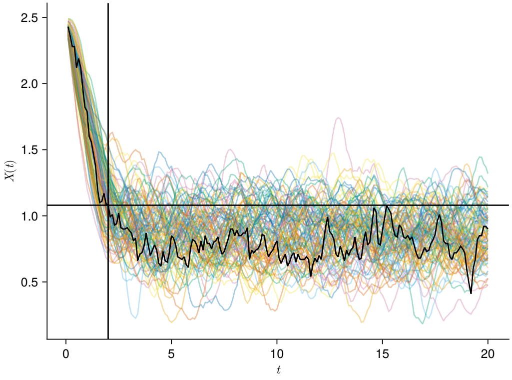




Actual Samples



Conditional, Generated Samples



Conclusions and Future Work

- Scalable to problems yet unseen in triangular transport
  - Improve implementation efficiency further
  - Tailor optimization to parameterizations
  - Improve GPU bindings
- Flexible for many use-cases without sacrificing performance
  - Allow user-specified functions and bases (e.g., Neural-net)
  - Incorporate built-in training for 'map-from-density'
- Easily apply maps or experiment with high-level transport algorithms
  - Incorporate fast quadrature for targets
- All presented materials are available at dsharp.dev/uq24

Conclusions and Future Work

- Scalable to problems yet unseen in triangular transport
  - Improve implementation efficiency further
  - Tailor optimization to parameterizations
  - Improve GPU bindings
- Flexible for many use-cases without sacrificing performance
  - Allow user-specified functions and bases (e.g., Neural-net)
  - Incorporate built-in training for ‘map-from-density’
- Easily apply maps or experiment with high-level transport algorithms
  - Incorporate fast quadrature for targets
- All presented materials are available at dsharp.dev/uq24

Conclusions and Future Work

- Scalable to problems yet unseen in triangular transport
  - Improve implementation efficiency further
  - Tailor optimization to parameterizations
  - Improve GPU bindings
- Flexible for many use-cases without sacrificing performance
  - Allow user-specified functions and bases (e.g., Neural-net)
  - Incorporate built-in training for ‘map-from-density’
- Easily apply maps or experiment with high-level transport algorithms
  - Incorporate fast quadrature for targets
- All presented materials are available at dsharp.dev/uq24