Data-driven reduced order models using invariant foliations, manifolds and autoencoders

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Contents

The assumptions

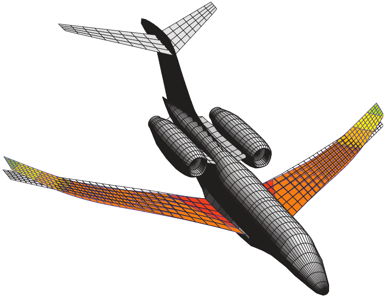


Diagram from: S. Preidikman & D. Mook, JVC, 2000

We have the data

$$(\boldsymbol{x}_k, \boldsymbol{y}_k)\,,\ k = 1, 2, \ldots, N \quad \boldsymbol{x}_k, \boldsymbol{y}_k \in \mathbb{R}^n$$

The data is approximately on the graph of function $\boldsymbol{F}$, i.e.,

$$\boldsymbol{y}_k = \boldsymbol{F}(\boldsymbol{x}_k) + \boldsymbol{\xi}_k,$$

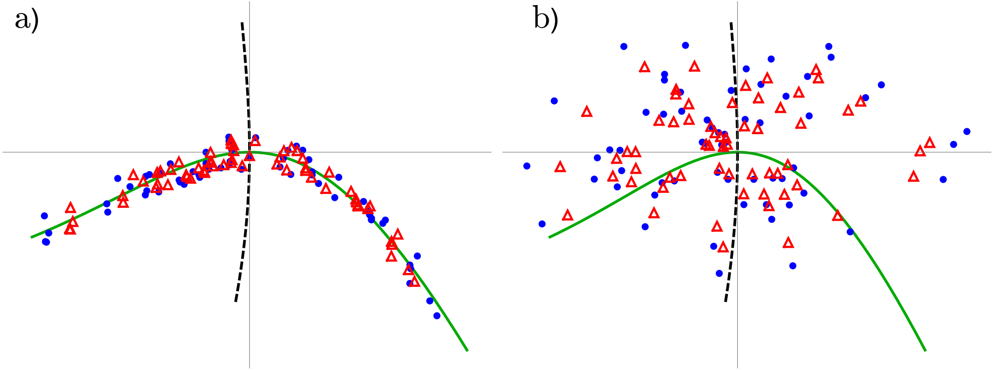
where $\boldsymbol{\xi}_k$ is a small random error with zero mean.

Find a low-dimensional description of the data

Create an abstraction, capture an invariant, etc...

Requirements

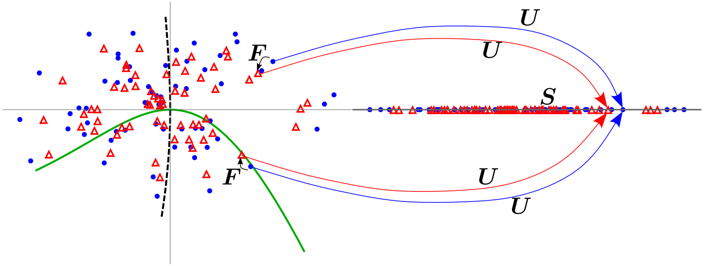
1. **Lower dimensional** than the manifold that the data covers



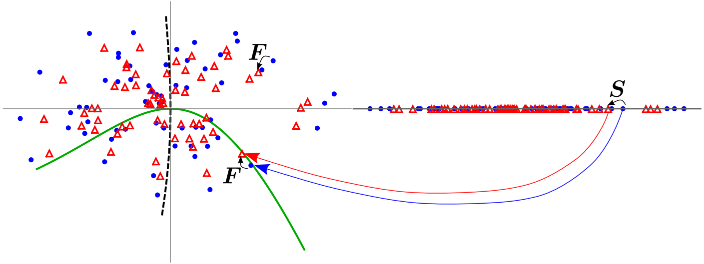
2. The data has a **connection** to the model
3. The model is unique, describes the data, predicts the future, explains phenomena, informs experimental design, etc

Connections to data

Two kinds of connections



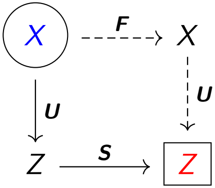
- Encoder (submersion)



- Decoder (immersion)

Four possibilies

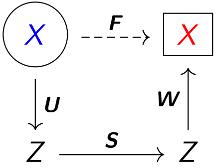
Invariant foliation



$$\boldsymbol{S}(\boldsymbol{U}(\boldsymbol{x})) = \boldsymbol{U}(\boldsymbol{F}(\boldsymbol{x}))$$

$$\boldsymbol{S}(\boldsymbol{U}(\boldsymbol{x}_k)) = \boldsymbol{U}(\boldsymbol{y}_k)$$

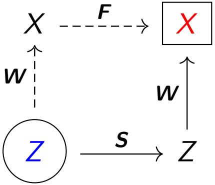
Autoencoder



$$\boldsymbol{W}(\boldsymbol{S}(\boldsymbol{U}(\boldsymbol{x}))) = \boldsymbol{F}(\boldsymbol{x})$$

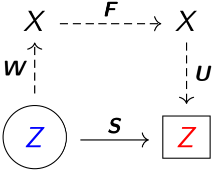
$$\boldsymbol{W}(\boldsymbol{S}(\boldsymbol{U}(\boldsymbol{x}_k))) = \boldsymbol{y}_k$$

Invariant manifold



$$\boldsymbol{W}(\boldsymbol{S}(\boldsymbol{z})) = \boldsymbol{F}(\boldsymbol{W}(\boldsymbol{z}))$$

Reverse autoencoder



$$\boldsymbol{S}(\boldsymbol{z}) = \boldsymbol{U}(\boldsymbol{F}(\boldsymbol{W}(\boldsymbol{z})))$$

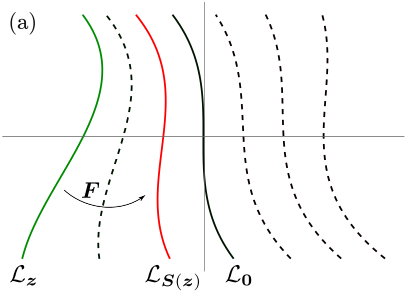
A weak definition of ROM: **invariance**

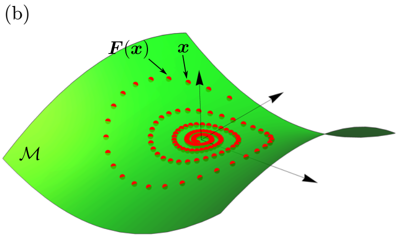
Definition

Assume two maps $\boldsymbol{F}: X \to X$, $\boldsymbol{S}: Z \to Z$ and a encoder $\boldsymbol{U}: X \to Z$ or a decoder $\boldsymbol{W}: Z \to X$.

1. The encoder-map pair $(\boldsymbol{U}, \boldsymbol{S})$ is a *reduced order model* (ROM) of $\boldsymbol{F}$ if for all initial conditions $\boldsymbol{x}_0 \in G \subset X$ the trajectory $\boldsymbol{x}_{k+1} = \boldsymbol{F}(\boldsymbol{x}_k)$ and for initial condition $\boldsymbol{z}_0 = \boldsymbol{U}(\boldsymbol{x}_0)$ the second trajectory $\boldsymbol{z}_{k+1} = \boldsymbol{S}(\boldsymbol{z}_k)$ are connected such that $\boldsymbol{z}_k = \boldsymbol{U}(\boldsymbol{x}_k)$ for all $k > 0$.
2. The decoder-map pair $(\boldsymbol{W}, \boldsymbol{S})$ is a *reduced order model* of $\boldsymbol{F}$ if for all initial conditions $\boldsymbol{z}_0 \in H = \{\boldsymbol{z} \in Z : \boldsymbol{W}(z) \in G\}$ the trajectory $\boldsymbol{z}_{k+1} = \boldsymbol{S}(\boldsymbol{z}_k)$ and for initial condition $\boldsymbol{x}_0 = \boldsymbol{W}(\boldsymbol{z}_0)$ the second trajectory $\boldsymbol{x}_{k+1} = \boldsymbol{F}(\boldsymbol{x}_k)$ are connected such that $\boldsymbol{x}_k = \boldsymbol{W}(\boldsymbol{z}_k)$ for all $k > 0$.

Invariant foliations and manifolds





A leaf is

$$\mathcal{L}_z = \{x \in G \subset X : U(x) = z\}$$

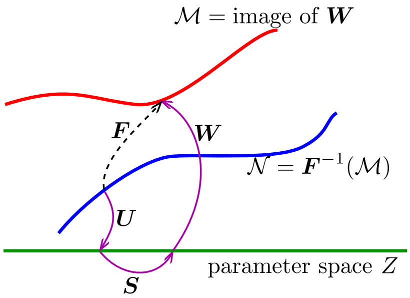
Invariance $F(\mathcal{L}_z) \subset \mathcal{L}_{S(z)}$ means

$$S(U(x)) = U(F(x))$$

Invariance is pointwise

$$W(S(z)) = F(W(z))$$

Autoencoder (or reverse autoencoder)



The connection says that

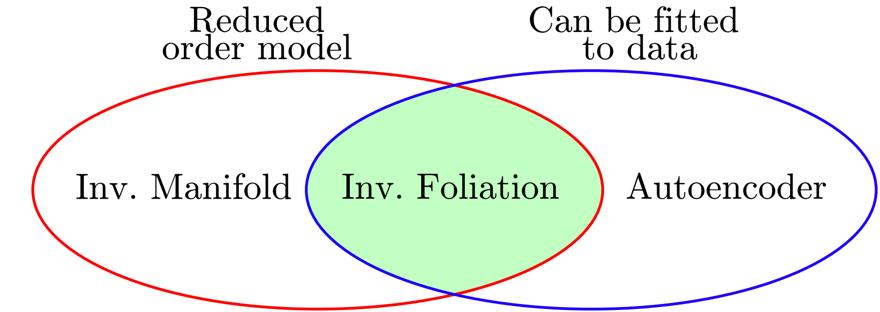
$$\boldsymbol{W}(\boldsymbol{S}(\boldsymbol{U}(\boldsymbol{x}))) = \boldsymbol{F}(\boldsymbol{x}) \quad \text{or} \quad \boldsymbol{S}(\boldsymbol{z}) = \boldsymbol{U}(\boldsymbol{F}(\boldsymbol{W}(\boldsymbol{z})))$$

Invariance occurs only if $\mathcal{M} \subset \mathcal{N}$. Or when

$$\sum_{k=1}^{N} \|\boldsymbol{W}(\boldsymbol{U}(\boldsymbol{x}_k)) - \boldsymbol{x}_k\|^2 \approx 0$$

All data must be on the manifold! $\implies$ Not a reduced order model

In summary



Reverse Autoencoder

Foliations: the smallprint of existence – uniqueness

Assume a steady state at $\boldsymbol{x} = 0$. Let μ_k be the eigenvalues of the Jacobian at the steady state, $\mu_1, \ldots, \mu_\nu$ correspond to the dynamics of interest.

Definition

The number

$$\beth_{E^\star} = \frac{\min_{k=1\ldots\nu} \log|\mu_k|}{\max_{k=1\ldots n} \log|\mu_k|}$$

is called the spectral quotient of the left-invariant linear subspace $E^\star$ of $\boldsymbol{F}$ about the origin.

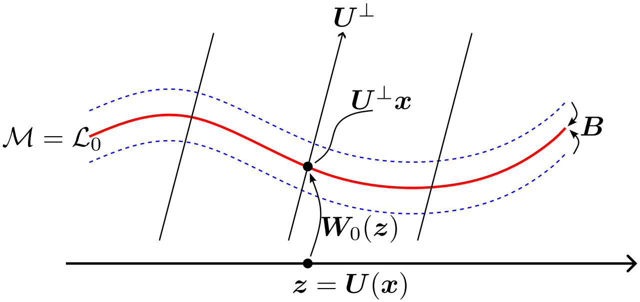
Theorem

Assume that $D\boldsymbol{F}(0)$ is semisimple and that there exists an integer $\sigma \geq 2$, such that $\beth_{E^\star} < \sigma \leq r$. Also assume that

$$\prod_{k=1}^{n} \mu_k^{m_k} \neq \mu_j,\ j = 1, \ldots, \nu \tag{1}$$

for all $m_k \geq 0$, $1 \leq k \leq n$ with at least one $m_l \neq 0$, $\nu + 1 \leq l \leq n$ and with $\sum_{k=0}^{n} m_k \leq \sigma - 1$. Then in a sufficiently small neighbourhood of the origin there exists an invariant foliation $\mathcal{F}$ tangent to the left-invariant linear subspace $E^\star$ of the C^r map $\boldsymbol{F}$. The foliation $\mathcal{F}$ is unique among the σ-times differentiable foliations and it is also C^r smooth.

Invariant manifolds as locally defined foliations



Define the encoder

$$\hat{U}(x) = U^\perp x - W_0(U(x))$$

In the neighbourhood of the invariant manifold

$$B\hat{U}(x) = \hat{U}(F(x))$$

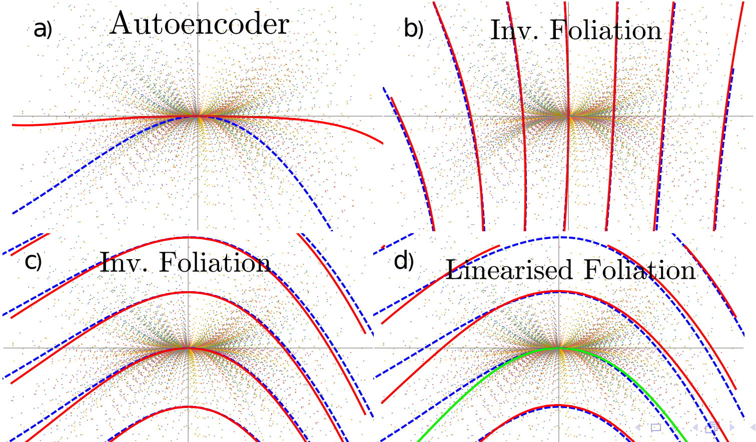
The decoder W is then reconstructed from $U^\perp$ and W_0.

A 2D example

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{V}\left(\boldsymbol{A}\boldsymbol{V}^{-1}(\boldsymbol{x})\right), \tag{2}$$

where

$$\boldsymbol{A} = \begin{pmatrix} \frac{9}{10} & 0 \\ 0 & \frac{4}{5} \end{pmatrix} \quad \boldsymbol{V}(\boldsymbol{x}) = \begin{pmatrix} x_1 + \frac{1}{4}\left(x_1^3 - 3(x_1 - 1)x_2x_1 + 2x_2^3 + (5x_1 - 2)x_2^2\right) \\ x_2 + \frac{1}{4}\left(2x_2^3 + (2x_1 - 1)x_2^2 - x_1^2(x_1 + 2)\right) \end{pmatrix}$$

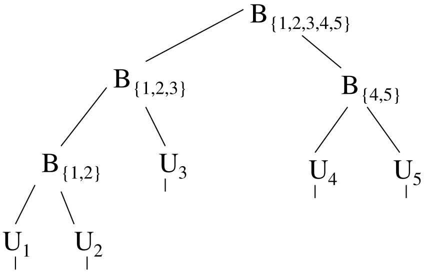


Tackling the curse of dimensionality: HT tensors

- The low-dimensional map $\boldsymbol{S}$ is a dense polynomial
- The **encoder** is a **compressed polynomial**

$$\boldsymbol{U}(\boldsymbol{x}) = \boldsymbol{U}^1 \boldsymbol{x} + \sum_{d=2}^{p} \sum_{i_1 \cdots i_d = 1}^{n} U_{t_r}^{d}(\cdot; i_1, \ldots, i_d)\, x_{i_1} \cdots x_{i_d},$$

$$d = 5, \mathbf{U}_i \in \mathbb{R}^{n \times k_i}, \mathbf{B}_t \in \mathbb{R}^{k_t \times k_{t_1} \times k_{t_2}}$$



- The tensor is defined recursively

$$U_t\left(p; i_1, \ldots, i_{|t_1|}, j_1, \ldots, j_{|t_2|}\right) =$$

$$= \sum_{q=1}^{k_{t_1}} \sum_{r=1}^{k_{t_2}} B_t(p, q, r)\, U_{t_1}\left(q; i_1, \ldots, i_{|t_1|}\right) U_{t_2}\left(r; j_1, \ldots, j_{|t_2|}\right),$$

(DNNs are hopeless for this application)

Ten-dimensional mechanical system

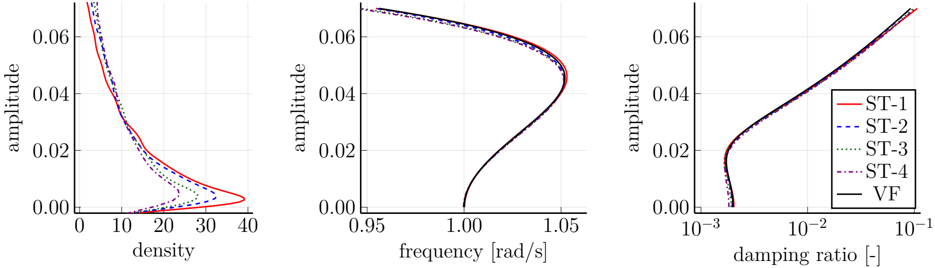
The system is a nonlinearly scrambled up version of

$$
\begin{aligned}
\dot r_1 &= -\tfrac{1}{500} r_1 + \tfrac{1}{100} r_1^3 - \tfrac{1}{10} r_1^5, \\
\dot r_2 &= -\tfrac{e}{500} r_2 - \tfrac{1}{10} r_2^5, \\
\dot r_3 &= -\tfrac{1}{50}\sqrt{\tfrac{3}{10}}\, r_3 + \tfrac{1}{100} r_3^3 - \tfrac{1}{10} r_3^5, \\
\dot r_4 &= -\tfrac{1}{500}\pi^2 r_4 + \tfrac{1}{100} r_4^3 - \tfrac{1}{10} r_4^5, \\
\dot r_5 &= -\tfrac{13}{500} r_5 + \tfrac{1}{100} r_5^3,
\end{aligned}
\qquad
\begin{aligned}
\dot\theta_1 &= 1 + \tfrac{1}{4} r_1^2 - \tfrac{3}{10} r_1^4, \\
\dot\theta_2 &= e + \tfrac{3}{20} r_2^2 - \tfrac{1}{5} r_2^4, \\
\dot\theta_3 &= \sqrt{30} + \tfrac{9}{50} r_3^2 - \tfrac{19}{100} r_3^4, \\
\dot\theta_4 &= \pi^2 + \tfrac{4}{25} r_4^2 - \tfrac{17}{100} r_4^4, \\
\dot\theta_5 &= 13 + \tfrac{4}{25} r_5^2 - \tfrac{9}{50} r_5^4.
\end{aligned}
$$

The transformations are $y_{2k-1} = r_k \cos\theta_k$ and $y_{2k} = r_k \sin\theta_k$ and then

$$
\begin{aligned}
y_1 &= z_1 + z_3 - \tfrac{1}{12} z_3 z_5, & y_2 &= z_2 - z_3, \\
y_3 &= z_3 + z_5 - \tfrac{1}{12} z_5 z_7, & y_4 &= z_4 - z_5, \\
y_5 &= z_5 + z_7 + \tfrac{1}{12} z_7 z_9, & y_6 &= z_6 - z_7, \\
y_7 &= z_7 + z_9 - \tfrac{1}{12} z_1 z_9, & y_8 &= z_8 - z_9, \\
y_9 &= z_9 + z_1 - \tfrac{1}{12} z_3 z_1, & y_{10} &= z_{10} - z_1,
\end{aligned}
$$

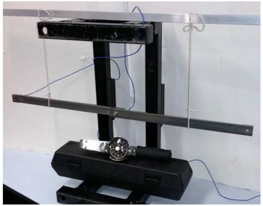
(a) (b) (c)

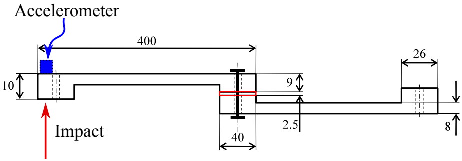


HT tensors max rank-6. Details: `https://arxiv.org/abs/2206.12269`

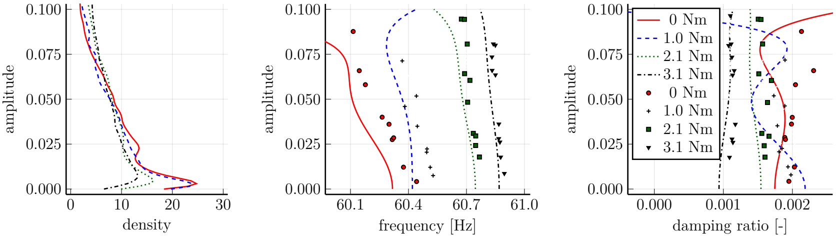
Jointed beam

(a) (b)

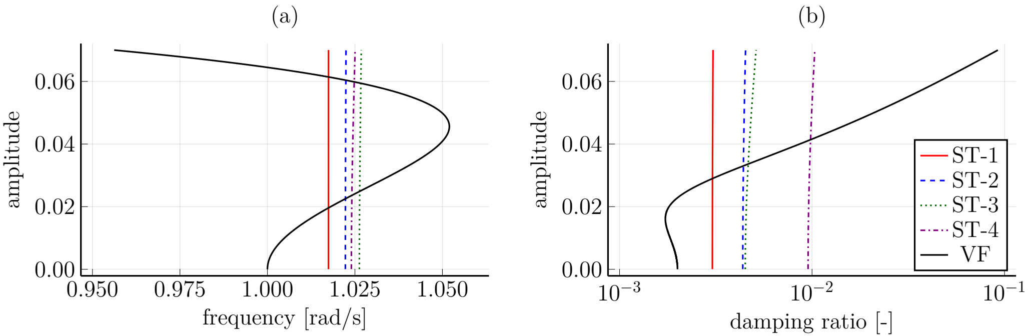




(a) (b) (c)



Comparing with Koopman

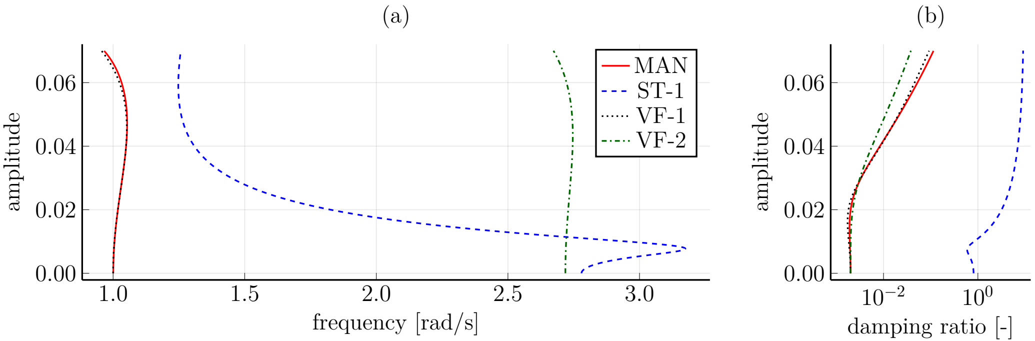


Disclaimer: tried to make the best out of it, but all comparions are unfair (apples vs. oranges)

Details: `https://arxiv.org/abs/2206.12269`

Software: `https://github.com/rs1909/FMA`

Comparing with SSMLearn – an autoencoder (Cenedese et al)



Disclaimer: tried to make the best out of it, but all comparions are unfair (apples vs. oranges)

Details: `https://arxiv.org/abs/2206.12269`

Software: `https://github.com/rs1909/FMA`

Conclusions

- Considered **all possibilies** for ROM identification
- Only **foliations** can be fitted to data and invariant at the same time
- Koopman is a special case of foliations, SSMLearn is an autoencoder, many others similarly just learn a manifold
- Try compressed tensors and Gauss-Southwell optimisation

Again, **many thanks** for the opportunity to speak!

Comparing with SSMLearn – an autoencoder (Cenedese et al)

A new parametrisation is needed: $\tilde{\boldsymbol{W}}(r,\theta) = \boldsymbol{W}(t,\theta+\delta(t))$, $t = \kappa^{-1}\left(\frac{r^2}{2}\right)$, where

$$\delta(r) = -\int_0^r \frac{\int_0^{2\pi}\langle D_1\boldsymbol{W}(\rho,\theta), D_2\boldsymbol{W}(\rho,\theta)\rangle_X \mathrm{d}\theta}{\int_0^{2\pi}\langle D_2\boldsymbol{W}(\rho,\theta), D_2\boldsymbol{W}(\rho,\theta)\rangle_X \mathrm{d}\theta}\mathrm{d}\rho,$$

$$\kappa(r) = \frac{1}{2\pi}\int_0^r \int_0^{2\pi} \langle D_1\boldsymbol{W}(\rho,\theta), \boldsymbol{W}(\rho,\theta)\rangle_X \mathrm{d}\theta\mathrm{d}\rho$$