数据驱动的降阶模型

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本堂课大纲

- 谱分解

- Koopman算子理论
  - Koopman算子的谱分解
  - Koopman模态

- Koopman算子近似算法
  - 动力学模态分解
  - 扩展动力学模态分解

谱分解

- 线性常微分方程

$$\frac{d}{dt}\boldsymbol{u}(t) = A\boldsymbol{u}(t)$$

- 基底选择

$$Av_k = \lambda_k v_k,\ k = 1,2\cdots\cdots,N$$

- 快速求解

$$\boldsymbol{u}(t) = \sum_k a_k(t) v_k$$

$$\frac{d}{dt}a_k(t) = \lambda_k a_k(t) \qquad a_k(t) = a_k(0)e^{\lambda_k t}$$

谱分解

- 线性常微分方程(离散时间)

$$\boldsymbol{u}(m+1) = A\boldsymbol{u}(m)$$

- 基底选择

$$Av_k = \lambda_k v_k,\ k = 1,2 \cdots\cdots, N$$

- 快速求解

$$\boldsymbol{u}(m) = \sum_k a_k(m) v_k$$

$$a_k(m+1) = \lambda_k a_k(m) \qquad a_k(m) = a_k(0)\lambda_k^m$$

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Koopman 算子

- 连续时间非线性模型

$$\frac{d}{dt}\boldsymbol{u} = f(\boldsymbol{u}) \quad \boldsymbol{u} \in \mathcal{M} \in R^N \qquad \mathcal{M}\text{是}N\text{维空间中流形}$$

半群：

$$F_t\colon \boldsymbol{u}(t_0) \to \boldsymbol{u}(t_0 + t) = \boldsymbol{u}(t_0) + \int_{t_0}^{t_0+t} f\big(\boldsymbol{u}(\tau)\big)d\tau$$

$$F_{t+s} = F_t \circ F_s$$

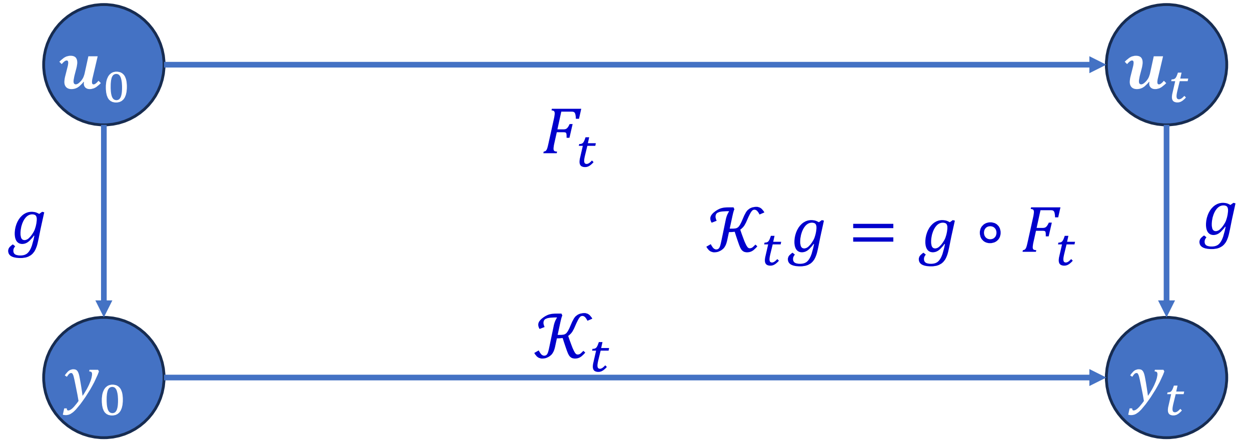
Koopman 算子

- Koopman算子(连续时间系统)

考虑由观测函数 g构成的空间$\mathfrak{G}$，Koopman算子$\mathcal{K}_t: \mathfrak{G} \rightarrow \mathfrak{G}$，满足

$$\mathcal{K}_t g = g \circ F_t$$

$$\frac{d}{dt}\boldsymbol{u} = f(\boldsymbol{u})$$



Koopman 算子

- Koopman算子(连续时间系统)

线性算子

$$\mathcal{K}_t(g+g') = (g+g')\circ F_t$$
$$= g\circ F_t + g'\circ F_t = \mathcal{K}_t g + \mathcal{K}_t g'$$

半群

$$\mathcal{K}_{t+s}g = g\circ F_{t+s} = g\circ(F_t\circ F_s)$$
$$= (g\circ F_t)\circ F_s = \mathcal{K}_t(g\circ F_s) = \mathcal{K}_t\mathcal{K}_s g$$

Koopman 算子

- 离散时间非线性模型

$$\boldsymbol{u}(m+1) = F(\boldsymbol{u}(m)) \in \mathcal{M} \in R^N \qquad \mathcal{M}\text{是}N\text{维空间中流形}$$

$$\boldsymbol{u}(m) = F^m(\boldsymbol{u}(0))$$

- Koopman算子(离散时间系统)

考虑由观测函数 g 构成的空间$\mathfrak{G}$，Koopman算子$\mathcal{K}$：$\mathfrak{G} \to \mathfrak{G}$，满足

$$\mathcal{K}g = g \circ F$$
$$\mathcal{K}^m g = g \circ F^m$$

Koopman 算子

Koopman算子是(无限维)线性算子

连续时间系统：$\mathcal{K}_t g = g \circ F_t$

离散时间系统：$\mathcal{K} g = g \circ F$

Koopman 算子的谱分解

- Koopman特征函数(连续时间系统)

无穷小生成元满足：

$$\mathcal{K}\varphi = \frac{d\mathcal{K}_t\varphi}{dt}\bigg|_{t=0} = \lim_{t\to 0}\frac{\mathcal{K}_t\varphi - \varphi}{t} = \lambda\varphi$$

对于观测函数φ

$$\mathcal{K}_t\varphi = \varphi \circ F_t = e^{\lambda t}\varphi$$

对于特征函数对(λ_1, φ_1)和(λ_2, φ_2)

$$\mathcal{K}[\varphi_1\varphi_2](u) = (\lambda_1 + \lambda_2)\varphi_1(u)\varphi_2(u)$$

$\Longrightarrow$特征函数对$(\lambda_1 + \lambda_2, \varphi_1\varphi_2)$

Koopman 算子的谱分解

➢ Koopman特征函数(连续时间系统)

例子：考虑非线性模型

$$\frac{du}{dt} = -u - u^3, u \in R$$

特征函数满足

$$\mathcal{K}\varphi(u) = \frac{d\mathcal{K}_t\varphi}{dt}\bigg|_{t=0}(u) = \nabla\varphi \cdot (-u - u^3) = \lambda\varphi$$

特征函数：

$$\varphi(u) = \frac{u}{\sqrt{1+u^2}} \quad \lambda = -1$$

$$\varphi_k(u) = \left(\frac{u}{\sqrt{1+u^2}}\right)^k \quad \lambda_k = -k$$

Koopman 算子的谱分解

- Koopman特征函数(离散时间系统)

对于观测函数φ

$$\mathcal{K}\varphi = \varphi \circ F = \lambda\varphi$$

对于特征函数对$(\lambda_1，\varphi_1)$和$(\lambda_2，\varphi_2)$

$$\begin{aligned}\mathcal{K}[\varphi_1\varphi_2](u) &= \varphi_1(Fu)\varphi_2(Fu)\\ &= \lambda_1\lambda_2\varphi_1(u)\varphi_2(u)\end{aligned}$$

$\Longrightarrow$特征函数对$(\lambda_1\lambda_2，\varphi_1\varphi_2)$

Koopman 算子的谱分解

- Koopman特征函数(离散时间系统)

例子：考虑线性模型

$$F(u) = Fu, u \in R^N$$

F的左特征值和特征向量满足

$$w_j^T F = \lambda_j w_j^T$$

Koopman算子的特征值和特征函数包含

$$\lambda_j, \varphi_j(u) = w_j^T u$$

$$\mathcal{K}\varphi_j(u) = \varphi_j(Fu) = w_j^T Fu = \lambda_j \varphi_j(u)$$

Koopman 模态（Modes）

- Koopman模态展开

给定Koopman算子的特征函数$\{\varphi_j\}_{j=1}^{\infty}$，对于观测函数

$$g = \sum_{j=1}^{\infty} v_j(g)\,\varphi_j$$

这些系数v_j称为与可观测函数g相关的Koopman模态。

连续时间系统：$\mathcal{K}_t g = \sum_{j=1}^{\infty} e^{\lambda_j t} \varphi_j\, v_j(g)$

离散时间系统：$\mathcal{K}^m g = \sum_{j=1}^{\infty} \lambda_j^m \varphi_j\, v_j(g)$

Koopman 模态（Modes）

- Koopman模态展开

考虑恒等观测量($id(\boldsymbol{u}) = \boldsymbol{u}$)

$$id = \sum_{j=1}^{\infty} v_j(id)\,\varphi_j$$

连续时间系统：

$$\boldsymbol{u}(t) = \mathcal{K}_t id(\boldsymbol{u}(0)) = \sum_{j=1}^{\infty} e^{\lambda_j t}\,\varphi_j(\boldsymbol{u}(0))v_j(id)$$

离散时间系统：

$$\boldsymbol{u}(m) = \mathcal{K}^m id(\boldsymbol{u}(0)) = \sum_{j=1}^{\infty} \lambda_j^m \varphi_j(\boldsymbol{u}(0))v_j(id)$$

Koopman 模态（Modes）

- 例子

考虑非线性系统

$$\dot{u}_1 = \mu u_1$$
$$\dot{u}_2 = \lambda(u_2 - u_1^2)$$

Koopman 算子

$$\mathcal{K} = \mu u_1 \frac{\partial}{\partial u_1} + \lambda(u_2 - u_1^2)\frac{\partial}{\partial u_2}$$

Koopman 算子的特征值和特征函数包含

$$\lambda_1 = \mu, \qquad \varphi_1(u) = u_1$$
$$\lambda_2 = \lambda, \qquad \varphi_2(u) = u_2 + \frac{\lambda}{2\mu-\lambda} u_1^2$$
$$\lambda_3 = 2\mu, \qquad \varphi_3(u) = u_1^2$$

我们有恒等算子

$$id(u) = \varphi_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \varphi_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \varphi_3 \begin{bmatrix} 0 \\ -\dfrac{\lambda}{2\mu - \lambda} \end{bmatrix}$$

Koopman 模态（Modes）

➢ 例子

考虑线性模型$\boldsymbol{u}_{k+1} = F\boldsymbol{u}_k \in R^N$

F的左右特征值和特征向量满足（假设$w_i^T v_j = \delta_{ij}$）

$$w_j^T F = \lambda_j w_j^T \quad F v_j = \lambda_j v_j$$

Koopman算子的特征值和特征函数包含$\{\lambda_j, \varphi_j(u) = w_j^T u\}$，$\{v_j\}$为恒等观测函数 id 相关的 Koopman 模式

$$id(\boldsymbol{u}(0)) = \sum_{j=1}^{N} v_j \varphi_j(\boldsymbol{u}(0))$$

我们有

$$\boldsymbol{u}(m) = \mathcal{K}^m id(\boldsymbol{u}(0)) = \sum_{j=1}^{\infty} \lambda_j^m v_j w_j^T \boldsymbol{u}(0)$$

Koopman 算子

Koopman算子是(无限维)线性算子

连续时间系统：$\mathcal{K}_t g = g \circ F_t$
离散时间系统：$\mathcal{K} g = g \circ F$

近似Koopman算子的谱和模态，能得到观测的演化

连续时间系统：$\boldsymbol{u}(t) = \sum_{j=1}^{\infty} e^{\lambda_j t} \varphi_j(\boldsymbol{u}(0))\, v_j(id)$
离散时间系统：$\boldsymbol{u}(m) = \sum_{j=1}^{\infty} \lambda_j^m \varphi_j\, (\boldsymbol{u}(0)) v_j(id)$

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Koopman 算子的近似

- 有限维近似

考虑观测函数 g 构成的空间 $\mathfrak{G}$ 的 N 维子空间

$$\mathfrak{G}_N \subset \mathfrak{G}$$

以及相应的投影映射 $\Pi: \mathfrak{G} \to \mathfrak{G}_N$

对于Koopman算子 $\mathcal{K}$，我们可以限制在 $\mathfrak{G}_N$ 上，定义

$$\mathcal{K}_N = \Pi \mathcal{K} \Big|_{\mathfrak{G}_N} : \mathfrak{G}_N \to \mathfrak{G}_N$$

用 $\mathcal{K}_N$ 来近似 $\mathcal{K}$。

动力学模态分解

- 投影映射$\Pi: \mathfrak{G} \to \mathfrak{G}_N$

  $\mathfrak{G}_N$的基底：$\Psi = [\psi_1\ \psi_2 \cdots\ \psi_N]$
  系数函数：Γ：$\mathfrak{G} \to C^N$
  $\Pi = \Psi\Gamma:\ g \to \Psi c\ \ (c = \Gamma g \in C^N)$
  $\Gamma\Psi = I$

- Koopman算子

$$\mathcal{K}_N g = \Pi\mathcal{K}\Pi g = \Psi\Gamma\mathcal{K}\Psi\Gamma g = \Psi K\Gamma g$$

其中

$$K: C^N \to C^N, \qquad Ka = \Gamma\mathcal{K}\Psi a$$

是$\mathcal{K}_N$的矩阵表示形式。它被称为系统的 Koopman 矩阵，并对应于 Koopman 运算符在坐标系 Ψ下对观测函数 g的作用。

动力学模态分解

- 数据收集

$$X = [\boldsymbol{u}(t_0) \quad \boldsymbol{u}(t_1) \quad \cdots\cdots \quad \boldsymbol{u}(t_{n-1})]$$
$$Y = [\boldsymbol{u}(t_1) \quad \boldsymbol{u}(t_2) \quad \cdots\cdots \quad \boldsymbol{u}(t_n)]$$
$$t_m = k\Delta t$$
$$\boldsymbol{u}(m) = \boldsymbol{u}(m\Delta t)$$

- Koopman算子

$$\mathcal{K}g(\boldsymbol{u}(m)) = g(\boldsymbol{u}(m+1))$$

- 动力学模态分解(Dynamic model decomposition)
  - $\mathfrak{G}_N$是$\boldsymbol{u}$在网格点的值，在x_i上的取值： $\psi_i(\boldsymbol{u})$
  - 找到最合适的K使得 $Y \approx KX$

动力学模态分解

➢ 动力学模态分解

目标：找到最合适的K使得 $Y \approx KX$

奇异值分解：$X = U\Sigma V^T$ $\Sigma \in R^{n\times n}$

Koopman矩阵：$K = YV\Sigma^{-1}U^T$

特征值、特征向量计算：

计算 $\tilde{K} := U^T YV\Sigma^{-1}$

$\tilde{K}$的特征值$\{\tilde{\lambda}_j\}$和左右特征向量$\{\tilde{w}_j\}\{\tilde{v}_j\}$，对应Koopman矩阵的特征值和左右特征向量

$$\lambda_j = \tilde{\lambda}_j$$

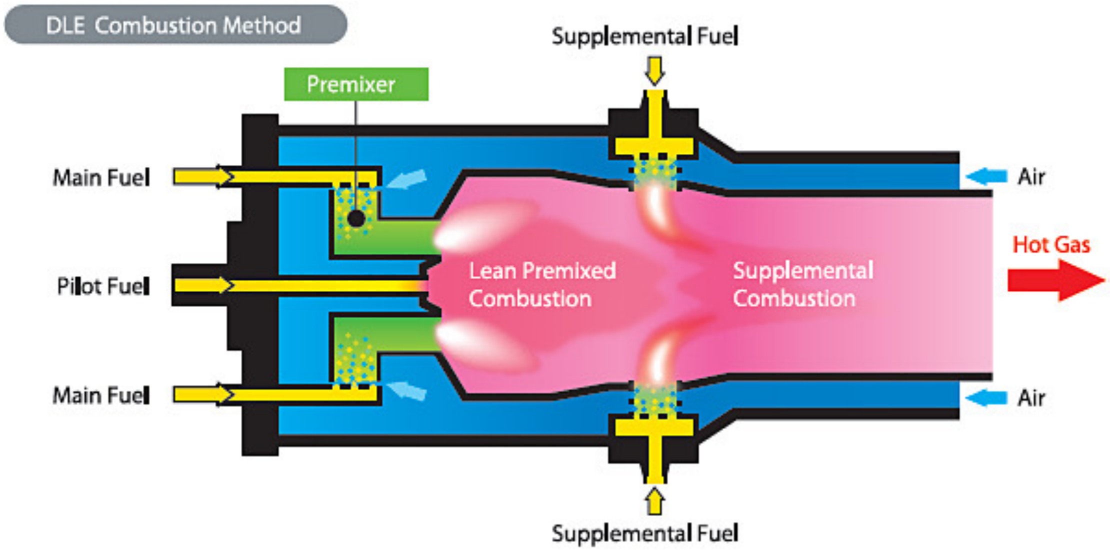
$$w_j = U\tilde{w}_j$$

$$v_j = YV\Sigma^{-1}\tilde{v}_j$$

复杂度：$\mathcal{O}(Nn^2)$

动力学模态分解

➢ 流体分析



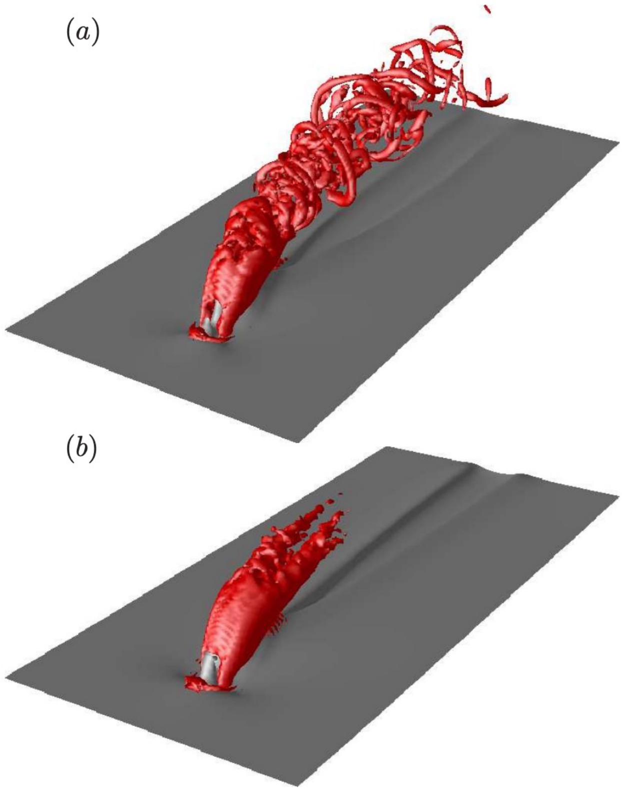
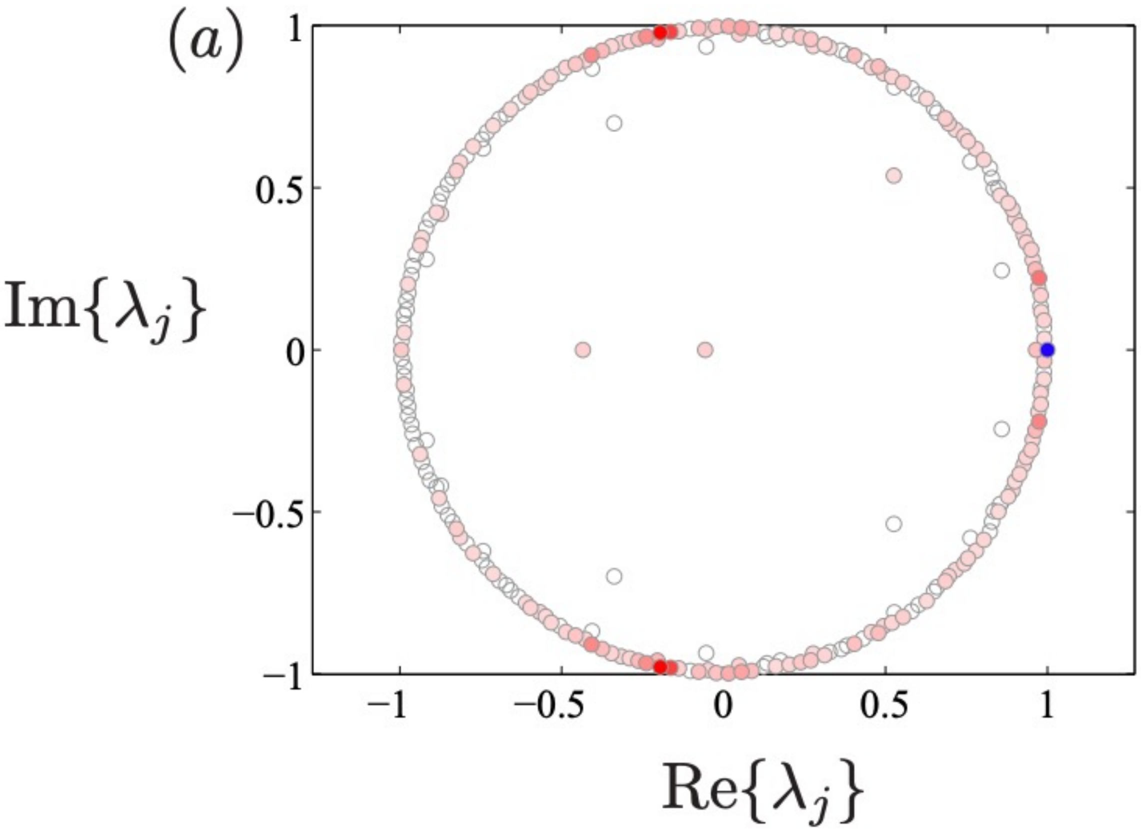


FIGURE 1. (a) Snapshot of the flow field at $t = 400$. Red and gray isocontours represent $\lambda_2 = -0.1$ and $u = 0.2$ (near the wall) respectively. (b) The same quantities for the time-averaged flow which also is the first Koopman mode.

动力学模态分解

➢ 流体分析



动力学模态分解

➢ 流体分析

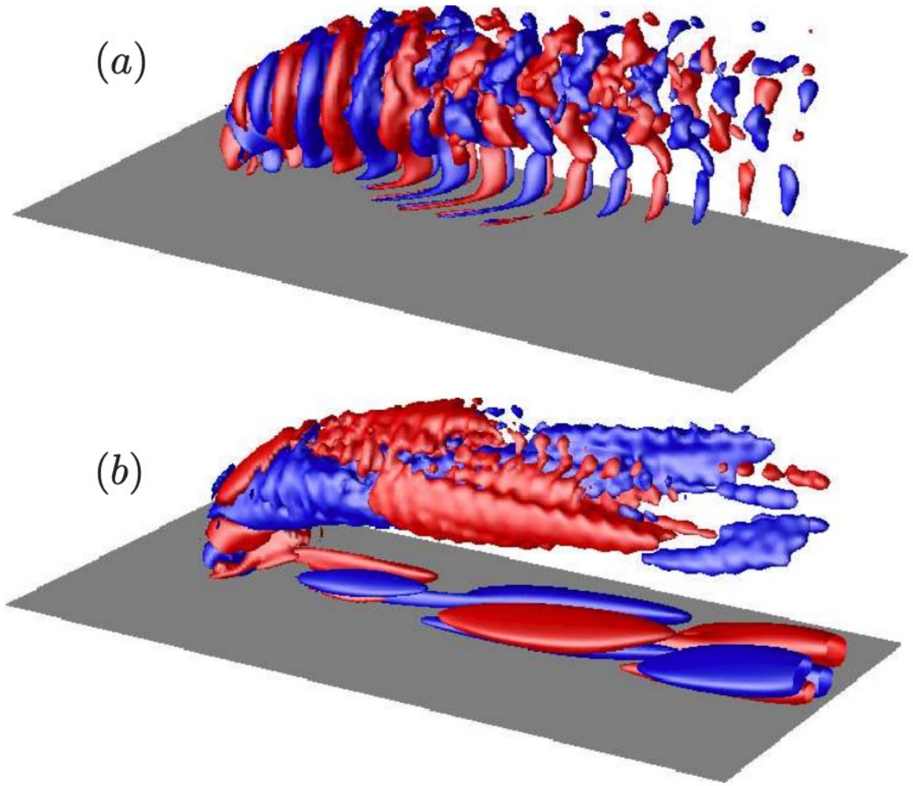


FIGURE 4. Positive (red) and negative (blue) contour levels of the streamwise velocity components of two Koopman modes. The wall is shown in gray. (a) Mode 2, with $\|\mathbf{v}_2\| = 400$ and $St_2 = 0.141$. (b) Mode 6, with $\|\mathbf{v}_6\| = 218$ and $St_6 = 0.0175$.

动力学模态分解

- 动力学模态分解

基于数据的模型：$\boldsymbol{u}(t_{m+1}) = K\boldsymbol{u}(t_m)$

快速求解：

$$\boldsymbol{u}(t_m) = \sum_{j=1} \lambda_j^m v_j w_j^T \boldsymbol{u}(t_0)$$

相比本征正交分解求得的基底，动力学模态分解求得的基底包含时序或是动力学信息。

扩展动力学模态分解

- 升维

用更多特征来近似Koopman算子

在$\mathcal{M}$上的函数空间中选择有限个的函数作为基函数：

$$\Psi = [\psi_1 ; \psi_2 ; \cdots\cdots ; \psi_D]$$

Koopman 算子近似：

$$\mathcal{K}_l g = \Pi \mathcal{K} \Pi g = \Psi \Gamma \mathcal{K} \Psi \Gamma g = \Psi K \Gamma g$$

其中

$$K: C^D \to C^D ，\qquad Ka = \Gamma \mathcal{K} \Psi a$$

$$\mathcal{K}\psi_i(\boldsymbol{u}) = \sum_{i=1}^{D} K_{i,j}\psi_j(\boldsymbol{u}) \quad K \in R^{D \times D}$$

扩展动力学模态分解

- 基函数选取

  傅里叶函数：$\psi(\boldsymbol{u}) = \langle \boldsymbol{u}, \sin 2\pi kx \rangle$

  多项式函数：$\psi(\boldsymbol{u}) = \langle \boldsymbol{u}, ax^2 + bx + c \rangle$

  高维函数：$\psi(\boldsymbol{u}) = \Pi_i f_i(\boldsymbol{u}_i)$

  基底函数：

$$\Psi = [\psi_1 \ \psi_2 \ \cdots\cdots \ \psi_l]$$

扩展动力学模态分解

- 扩展动力学模态分解

$$X = [\Psi(\boldsymbol{u}_0)\ \Psi(\boldsymbol{u}_1) \cdots\cdots\ \Psi(\boldsymbol{u}_{n-1})] \in R^{D\times n}$$
$$Y = [\Psi(\boldsymbol{u}_1)\ \Psi(\boldsymbol{u}_2) \cdots\cdots\ \Psi(\boldsymbol{u}_{n})] \in R^{D\times n}$$
$$Y \approx KX$$

- 谱分解

K的特征值$\{\lambda_j\}$和左特征向量$\{w_j\}$，对应Koopman算子的特征值$\{\lambda_j\}$和特征向量$\{w_j^T\Psi\}$

$$\mathcal{K}\left(w_j^T\Psi\right) \approx w_j^T K\Psi = \lambda_j w_j^T \Psi$$

- Koopman模态

$$\mathrm{id}(\boldsymbol{u}) = \sum_{j=1}^{D} w_j^T \Psi(\boldsymbol{u}) v_j \qquad F^{(m)}(\boldsymbol{u}) = \sum_{j=1}^{D} \lambda_j^m w_j^T \Psi(\boldsymbol{u}) v_j$$

扩展动力学模态分解

- 计算特征值、特征向量

Koopman矩阵：$K = Y(X^TX)^{-1}X^T$

计算特征值和左特征向量

$$w_j^T K = \lambda_j w_j^T$$

- 计算Koopman模态

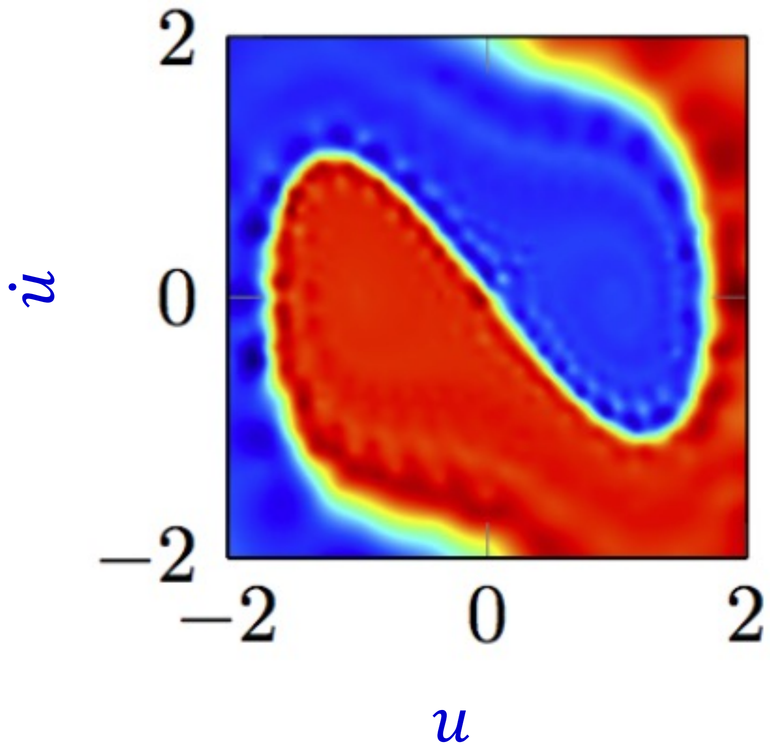
$$id(\boldsymbol{u}) = \sum_{j=1}^{D} w_j^T \Psi(\boldsymbol{u}) v_j$$

$$[\boldsymbol{u}_0\ \boldsymbol{u}_1, \cdots\ \boldsymbol{u}_{n-1}] = [v_1, v_2, \cdots, v_D] \begin{bmatrix} w_1^T \\ w_2^T \\ \vdots \\ w_D^T \end{bmatrix} [\Psi(\boldsymbol{u}_0)\Psi(\boldsymbol{u}_1)\cdots\Psi(\boldsymbol{u}_{n-1})]$$

扩展动力学模态分解

- 无强迫Duffing振荡器

$$\ddot{u} = -\delta\dot{u} - u(\beta + \alpha u^2) \qquad (\delta = 0.5, \alpha = 1, \beta = -1)$$



薄板样条： $\psi_i = r_i^2 \log(r_i^2)$， $r_i^2 = (u - x_i)^2 + (\dot{u} - y_i)^2$

扩展动力学模态分解

- 核函数

$$\Psi = [\psi_1\ \ \psi_2\ \cdots\cdots\ \psi_D] \qquad \Psi(x)^T\Psi(y) = \kappa(x,y)$$

$$X = [\Psi(\boldsymbol{u}_0)\ \Psi(\boldsymbol{u}_1)\cdots\cdots\ \Psi(\boldsymbol{u}_{n-1})] \in R^{D\times n}$$
$$Y = [\Psi(\boldsymbol{u}_1)\ \Psi(\boldsymbol{u}_2)\cdots\cdots\ \Psi(\boldsymbol{u}_n)] \in R^{D\times n} \qquad Y \approx KX$$

$$X^TY = \begin{bmatrix} \kappa(\boldsymbol{u}_0,\boldsymbol{u}_1) & \kappa(\boldsymbol{u}_0,\boldsymbol{u}_2) & \cdots & \kappa(\boldsymbol{u}_0,\boldsymbol{u}_n) \\ \kappa(\boldsymbol{u}_1,\boldsymbol{u}_1) & \kappa(\boldsymbol{u}_1,\boldsymbol{u}_2) & \cdots & \kappa(\boldsymbol{u}_1,\boldsymbol{u}_n) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_1) & \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_2) & \cdots & \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_n) \end{bmatrix}$$

$$X^TX = \begin{bmatrix} \kappa(\boldsymbol{u}_0,\boldsymbol{u}_0) & \kappa(\boldsymbol{u}_0,\boldsymbol{u}_1) & \cdots & \kappa(\boldsymbol{u}_0,\boldsymbol{u}_{n-1}) \\ \kappa(\boldsymbol{u}_1,\boldsymbol{u}_0) & \kappa(\boldsymbol{u}_1,\boldsymbol{u}_1) & \cdots & \kappa(\boldsymbol{u}_1,\boldsymbol{u}_{n-1}) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_0) & \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_1) & \cdots & \kappa(\boldsymbol{u}_{n-1},\boldsymbol{u}_{n-1}) \end{bmatrix}$$

扩展动力学模态分解

➢ 计算特征值、特征向量

Koopman矩阵：$X^TX = V\Sigma^2V^T \ \ (X = U\Sigma V^T)$

$$K = YV\Sigma^{-1}U^T$$

$$\widetilde{K} = U^TKU = \Sigma^{-1}V^TX^TYV\Sigma^{-1}$$

$\widetilde{K}$的特征值和左特征向量满足

$$\widetilde{w}_j^T\widetilde{K} = \tilde{\lambda}_j\widetilde{w}_j^T$$

那么K的特征值和左特征向量满足

$$w_j^TK = \lambda_jw_j^T$$

其中$\lambda_j = \tilde{\lambda}_j \quad w_j^T = \widetilde{w}_j^TU^T$

扩展动力学模态分解

➢ 计算Koopman模态

$$id(\boldsymbol{u}) = \sum_{j=1}^{D} w_j^T \Psi(\boldsymbol{u}) v_j$$

$$[\boldsymbol{u}_0\ \boldsymbol{u}_1, \cdots\ \boldsymbol{u}_{m-1}] = [v_1, v_2, \cdots, v_D] \begin{bmatrix} w_1^T \\ w_2^T \\ \vdots \\ w_D^T \end{bmatrix} X$$

$$= [v_1, v_2, \cdots, v_D] \begin{bmatrix} \widetilde{w}_1^T \\ \widetilde{w}_2^T \\ \vdots \\ \widetilde{w}_D^T \end{bmatrix} \Sigma V^T$$

扩展阅读

➢ 文献

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