SPARSE COLLOCATION METHODS

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- Consider the dynamical system driven by Gaussian white noise

$$d\mathbf{x}(t) = f(\mathbf{x}(t),t)dt + G(\mathbf{x}(t),t)d\beta(t)$$
$$\mathrm{E}[d\beta(t)\beta^T(t)] = \mathbf{Q}(t)dt \qquad p(\mathbf{x}(t_0)) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$$

- The time-evolution of the state PDF is given by the FPKE:

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = \mathcal{L}_{\mathcal{FP}}(p(\mathbf{x},t))$$
$$= \sum_{i=1}^{n} \frac{\partial (pf_i)}{\partial x_i} + \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial^2 \left[\left(\mathbf{GQG}^T\right)_{ij} p \right]}{\partial x_i \partial x_j}$$

SOLUTION CONSTRAINTS

1. Positivity of the PDF: $p(\mathbf{x},t) \geq 0 \quad \forall \mathbf{x}, t$.
2. Infinite Boundary Conditions of the PDF: $p(t, \pm\infty) = 0$
3. Normality of the PDF: $\int p(\mathbf{x},t)d\mathbf{x} = 1$.

- The positivity constraint can be circumvented by assuming the PDF has the form:
$$p(\mathbf{x},t) = e^{\beta(\mathbf{x},t)} \tag{1}$$
- To enforce the infinite boundary conditions constraint, the true PDF is regularized by a weighting function:
  - $p_A(\mathbf{x},t) = p(\mathbf{x},t)W(\mathbf{x},t,\boldsymbol{\theta}) = e^{(\beta(\mathbf{x},t)+\beta_W(\mathbf{x},t,\boldsymbol{\theta}))} = e^{\beta_A(\mathbf{x},t,\theta)}$
  - $W(\mathbf{x},t,\boldsymbol{\theta}) \geq 0 \quad \forall \mathbf{x},t,\boldsymbol{\theta}$.
  - $W(-\infty,t,\boldsymbol{\theta}) = W(\infty,t,\boldsymbol{\theta}) = 0 \quad \forall t,\boldsymbol{\theta}$.
- The weight function can be assumed to be a Gaussian function and constructed from the propagation of quadrature points:

$$\beta_W(\mathbf{x},t,\boldsymbol{\theta}) = \log\left[\frac{1}{\sqrt{|2\pi\boldsymbol{\Sigma}(t)|}}\right] - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}(t))^T\boldsymbol{\Sigma}(t)^{-1}(\mathbf{x}-\boldsymbol{\mu}(t)) \tag{2}$$

Residual Error: Resulting log-PDF Equation

$$e(\mathbf{x},t) = -\dot{\beta}_A(\mathbf{x},t,\boldsymbol{\theta}) - \frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}^T \dot{\boldsymbol{\theta}} - \mathbf{f}^T(\mathbf{x},t)\left[\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \mathbf{x}} + \frac{\partial \boldsymbol{\theta}}{\partial \mathbf{x}}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right]$$
$$-Tr\left[\frac{\partial \mathbf{f}(\mathbf{x},t)}{\partial \mathbf{x}}\right] + \frac{1}{2}Tr\Bigg[\mathbf{g}(t)\mathbf{Q}(t)\mathbf{g}^T(t)\Bigg(\frac{\partial^2 \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \mathbf{x}\partial \mathbf{x}^T} + \frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \mathbf{x}}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \mathbf{x}^T}$$
$$+2\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \mathbf{x}}\left(\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{x}}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^T + \frac{\partial^2 \boldsymbol{\theta}}{\partial \mathbf{x}\partial \mathbf{x}^T}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} + \frac{\partial^2 \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}\partial \mathbf{x}^T}\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{x}}$$
$$+\left(\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{x}}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)\left(\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{x}}\frac{\partial \beta_A(\mathbf{x},t,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right)^T\Bigg)\Bigg]$$

- A truncated expansion is used to approximate the state PDF:

$$\beta_A(\mathbf{x},t) = \beta(\mathbf{x},t) + \beta_W(\mathbf{x},\boldsymbol{\theta}) = \underbrace{\mathbf{c}(t)^T}_{unknown}\ \Phi(\mathbf{x}) + \mathbf{c}_W^T\Phi(\mathbf{x}) \quad (3)$$

- **Method of Weighted Residuals:** Residual error projected onto set of mutually-independent weight functions.

$$\int_{\Omega} \psi_j(\mathbf{x}) e(\mathbf{x}, t) = 0, \quad j = 1, 2, \cdots, m \tag{4}$$

- **Method of Weighted Residuals:** Residual error projected onto set of mutually-independent weight functions.

$$\int_{\Omega} \psi_j(\mathbf{x}) e(\mathbf{x},t) = 0, \quad j = 1,2,\cdots,m \tag{4}$$

- **Galerkin Method:** $\psi_j(\mathbf{x}) = \phi_j(\mathbf{x})$.
- **Least-Squares:** $\psi_j(\mathbf{x}) = \frac{\partial e(\mathbf{x},t)}{\partial c_j}$.
- **Collocation Method:** $\psi_j(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_j)$.

All these methods results in m equations for m unknowns.

- Collocation ODE: $\mathbf{A}\frac{\mathbf{c}_{k+1}-\mathbf{c}_k}{\Delta t}+\mathbf{B}+\mathbf{D}(\mathbf{c}_k)=0$

$$\mathbf{A}_j = \Phi(\mathbf{x}_j)^T \tag{5}$$

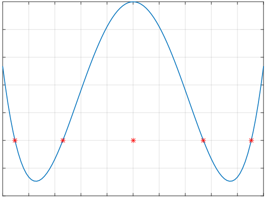
$$\begin{aligned}\mathbf{B}_j =& Tr\left[\frac{\partial \mathbf{f}(t_k,\mathbf{x})}{\partial \mathbf{x}}\right]_{\mathbf{x}=\mathbf{x}_j} \\ &+ \mathbf{f}(\mathbf{x}_j,t_k)^T\left[\frac{\partial \Phi(\mathbf{x})}{\partial \mathbf{x}}^T(\mathbf{c}_k+\mathbf{c}_W)\right]_{\mathbf{x}=\mathbf{x}_j}\end{aligned} \tag{6}$$

$$\begin{aligned}\mathbf{D}_j(\mathbf{c}_k) =& -\frac{1}{2}Tr\Bigg[\mathbf{G}\mathbf{Q}_p(t)\mathbf{G}^T \\ &\cdot\Bigg((\mathbf{c}_k+\mathbf{c}_W)^T\frac{\partial \Phi(\mathbf{x})}{\partial \mathbf{x}}\frac{\partial \Phi(\mathbf{x})}{\partial \mathbf{x}^T}(\mathbf{c}_k+\mathbf{c}_W) \\ &+\frac{\partial^2}{\partial \mathbf{x}\partial \mathbf{x}^T}\left[(\mathbf{c}_k+\mathbf{c}_W)^T\Phi(\mathbf{x})\right]\Bigg)\Bigg]_{\mathbf{x}=\mathbf{x}_j}\end{aligned} \tag{7}$$

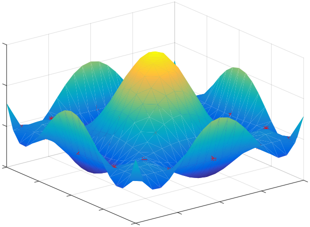
- In $1-D$, optimal choice is:
  - Collocation Points: Gaussian quadrature points.
  - Basis Functions: Lagrange Interpolation polynomials.

$$\phi(x) = \sum_{i=1}^{N}\left(y_i \prod_{k=1,k\neq i}^{N} \frac{x-x_i}{x_i-x_k}\right)$$

- In multidimensional systems, tensor product is required for Gaussian quadrature points and Lagrange Polynomials.



(a) 4^{th} Order Lagrange Poly: $1-D$



(b) 8^{th} Order Lagrange Poly: $2-D$

- Tensor product of quadrature points:
  - Exponential growth ($N = q^d$).
- Lagrange Interpolation polynomials in $d-$dimensional space:
  - Very high order basis set $\rightarrow$ Runge/Gibbs Phenomenon.
  - Tensor product of second-order polynomials results in one fourth-order polynomial in $2-D$.
- Standard polynomial basis set:
  - n^{th} order polynomial basis set $\rightarrow$ combinatorial growth $\binom{n+d}{d}$.
  - Fully-determined system is desired.
  - In general, $\binom{n+d}{d} \neq q^d$.

Main Challenge

# of basis function $\neq$ # of collocation points.

- **Over-Determined System:** # of basis functions $(m) <$ # of collocation points $(N) \rightarrow$ No Solution!
- **Under-Determined System:** # of basis functions $(m) >$ # of collocation points $(N) \rightarrow$ Infinitely Many Solutions!

Basis Functions for a given set of collocation points.

- *Least/Minimal degree interpolation*, active area of research.
- Find the set of monomials of least degree that are 'suitable' for the given collocation points.
- Form the *Vandermonde Matrix*, columns consists of monomials of increasing order, and each row corresponds to evaluation at one point
- Perform *Gauss elimination* with partial pivoting (based on specific rules).

$V(\mathbf{x}) = \sum_{i=0}^{m} c_i \phi_i(\mathbf{x}) = \mathbf{c}^T \phi(\mathbf{x})$

$Given\ V_j, \rightarrow find\ c_i$

Known basis functions of increasing degree →

$$\bar{\mathbf{V}} = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_N \end{bmatrix} = \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \dots & \phi_m(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \dots & \phi_m(\mathbf{x}_2) \\ \vdots & \vdots & \dots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \dots & \phi_m(\mathbf{x}_N) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = A_{N\times m}\mathbf{c}_{m\times 1}$$

Known function values at the points

Vandermonde Matrix → $A_{N\times m}$

Unknown coefficients

Fewer points than the number of basis functions N<m

Proposed Approach : $Sparse\ l_1 - norm\ optimization$

Convex Optimization !! →

$$\min_{c} : \quad \|\mathbf{c}\|_1$$
$$subject\ to : \quad A\mathbf{c} = V$$

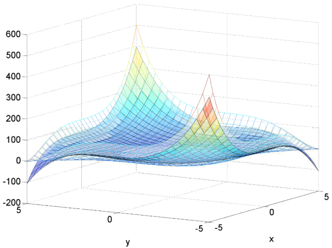
- Ideally, $l_0 - norm$ optimization selects the optimal coefficients and makes the remaining to 0 → *Non-convex*

Example: We want to interpolate the known polynomial function:

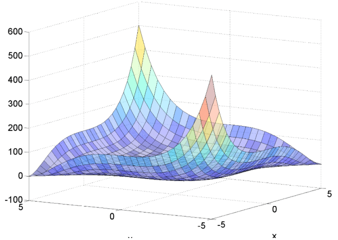
$$p(x) = (3x_1^3 + 2x_1^2 x_2 + 2x_1 x_2^2 + 5x_2^3 + 8x_1^6 + 16x_1^3 x_2^3 + 8x_2^6)/10^3$$

- Choice of interpolation points : Gauss-Legendre with 4 points in each dimension → 16 points in total for this 2D function
- Choice of polynomial basis : All polynomials/monomials up to degree 6 → 28 basis functions in total
- Excess of 12 basis functions, that need to be eliminated
- Get the function value at the interpolation points x_i → $V_i = p(x_i)$
- Form the under-determined system $V = Ac$
- Compare *Least-degree interpolation* to *sparse optimization based interpolation*

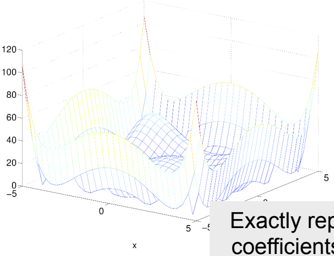
Collocation Approach
Sparse Approximation

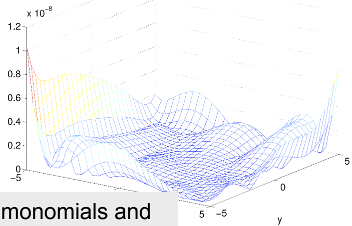


Least-degree interpolation error ~ 106.122



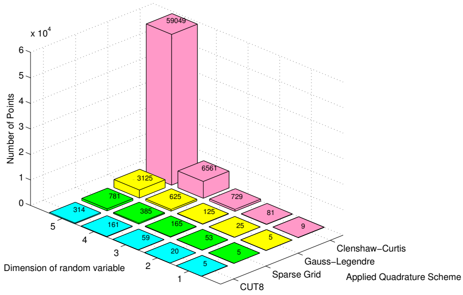
Sparse interpolation error ~ 1.03×10^{-8}



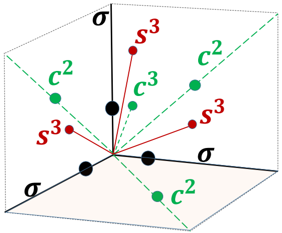


Exactly reproduces the monomials and coefficients of the original function with

Collocation Approach
Collocation Points



(c) CUT Comparison



(d) CUT Points in 3D

- The Conjugate Unscented Transform (CUT) → non-product, minimal cubature rules.
- CUT originally developed to compute desired-order polynomial function (expectation) integrals with the same accuracy as Gaussian quadrature methods.

- Convex optimization problem:

$$\text{Sparsity Condition:} \quad \min_{\mathbf{c}_{k+1}} \quad ||\mathbf{K}\mathbf{c}_{k+1}||_1 \tag{8}$$

subject to:

$$\text{Collocation:} \quad \mathbf{A}\mathbf{c}_{k+1} = \mathbf{A}\mathbf{c}_k - \Delta t\mathbf{B} - \Delta t\mathbf{D}(\mathbf{c}_k) \tag{9}$$

- An iterative l_1 optimization routine is proposed to optimally select the required basis functions to obtain a sparse, minimal polynomial expression for the log-PDF.
- Minimal set of collocation points generated via CUT.
- Number of non-contributing basis functions is lower-bounded by $m-N$.

Algorithm 1: Iterative Weighted l_1 optimization: $c^*_{k+1} = WeightedOpt(\mathbf{K}, \mathbf{c}_k, \mathbf{c}_W, \mathbf{A}, \mathbf{B}, \mathbf{D}(c_k), m, N, \Delta t, \varepsilon)$

Data: $\mathbf{K}$, $\mathbf{c}_k$, $\mathbf{c}_W$, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{D}(c_k)$, m, N, Δt, ε

Result: c^*_{k-1} with at least $m-N$ components set equal to zero

$\mathscr{C} = \varnothing$

$$\mathbf{c}^*_{k+1} = arg \min_{\mathbf{c}_{k+1}} \|\mathbf{K}\mathbf{c}_{k+1}\|_1$$
$$\text{Subject to: } \mathbf{A}\mathbf{c}_{k+1} = \mathbf{A}(\mathbf{c}_k) - \Delta t \mathbf{B}\mathbf{c}_k - \Delta t \mathbf{D}(\mathbf{c}_k)$$

$\mathscr{C} = \mathscr{C} \cup index\{c^*_{k+1} = 0\}$

if $card(\mathscr{C}) \geq m-N$ **then**

  Return $\mathbf{c}^*_{k+1}$.

else

  while $card(\mathscr{C}) < m-N$ **do**

    $\mathbf{K} = 1/(c^*_{k+1} + \varepsilon)$

$$\mathbf{c}^*_{k+1} = arg \min_{\mathbf{c}_{k+1}} \|\mathbf{K}\mathbf{c}_{k+1}\|_1$$
$$\text{Subject to: } \mathbf{A}\mathbf{c}_{k+1} = \mathbf{A}(\mathbf{c}_k) - \Delta t \mathbf{B}\mathbf{c}_k - \Delta t \mathbf{D}(\mathbf{c}_k)$$

    $\mathscr{C} = \mathscr{C} \cup index\{c^*_{k+1} = 0\}$

Algorithm 2: Collocation-Based Solution of the Fokker-Planck-Kolmogorov Equation

Data: $\mathbf{f}(\mathbf{x})$, $\mathbf{G}(\mathbf{x})$, m basis $\phi(\mathbf{x})$, initial values of coefficients $\mathbf{c}_0$, weight function coefficients $\mathbf{c}_W$, discretized time vector t, time step Δt, collocation points X_i $i = 1, 2, \ldots, N$, initial weight matrix $\mathbf{K}_0$, and weight update parameter ε.

Result: $\beta(\mathbf{x}, t)$.

Set $\mathbf{K} = \mathbf{K}_0$.

Compute matrix $\mathbf{A}$.

for $t = 0$, $t \leq t_f$, $k = k+1$ **do**

- Compute $\mathbf{B}$, $\mathbf{D}$ and $\mathbf{F}$ using $\mathbf{c}_k$.
- $\mathbf{c}_{k+1} = WeightedOpt(\mathbf{K}, \mathbf{c}_k, \mathbf{c}_W, \mathbf{A}, \mathbf{B}, \mathbf{D}(\mathbf{c}_k), m, N, \Delta t, \varepsilon)$.
- $\beta(k+1, \mathbf{x}) = (\mathbf{c}_{k+1} + \mathbf{c}_W)^T \Phi(\mathbf{x})$.

- Map global domain to unit hypercube via linear transformation.

$$\mathbf{y} = \mathbf{T}(\mathbf{x} + \mathbf{B}_0) \tag{10}$$

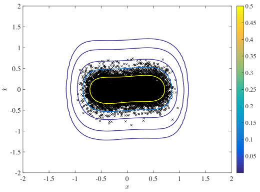
- Map system dynamics and Jacobian to local space:

$$\dot{\mathbf{y}} = \bar{\mathbf{f}}(\mathbf{y}, t) + \bar{\mathbf{G}}\Gamma(t) \tag{11}$$

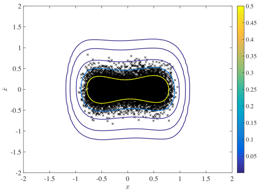
- Collocation points mapped to local space.
- Basis set generated in local space.
    - Simple to re-write FPKE in local space directly using mapped dynamics.
- Solution in local domain can be mapped to global domain:

$$p(\mathbf{x}, t) = p(\mathbf{y} = \mathbf{T}(\mathbf{x} + \mathbf{B}_0), t) \left| \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right| \tag{12}$$

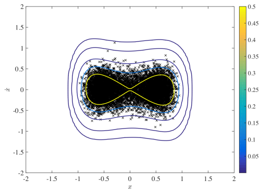
1. Duffing Oscillator.
   - $t_f = 100$ *sec*. with $\Delta t = 0.01$ *sec*.
   - CUT8-G: $\boldsymbol{\mu} = 0$, $\boldsymbol{\Sigma} = \text{diag}\,[0.125,\ 0.05] \rightarrow N = 21$.
   - Polynomials up to and including 15^{th} order $\rightarrow m = 136$.
   - Global domain: $\mathbf{x} \in [-2, 2] \rightarrow \mathbf{T} = \frac{1}{2}\mathbf{I}_{2\times 2}$.
2. Van-der-Pol Oscillator.
   - $t_f = 20$ *sec*. with $\Delta t = 0.01$ *sec*.
   - CUT8-G: $\boldsymbol{\mu} = 0$, $\boldsymbol{\Sigma} = 1.25\mathbf{I}_{2\times 2} \rightarrow N = 21$.
   - Polynomials up to and including 15^{th} order $\rightarrow m = 136$.
   - Global domain: $\mathbf{x} \in [-5, 5] \rightarrow \mathbf{T} = \frac{1}{5}\mathbf{I}_{2\times 2}$.
3. Quintic Oscillator.
   - $t_f = 100$ *sec*. with $\Delta t = 0.01$ *sec*.
   - CUT8-U on $\mathbf{x} \in [\pm 1.25, \pm 0.75] \rightarrow N = 21$.
   - Polynomials up to and including 10^{th} order $\rightarrow m = 66$.
   - Global domain: $\mathbf{x} \in [-2, 2] \rightarrow \mathbf{T} = \frac{1}{2}\mathbf{I}_{2\times 2}$.



(a) $t=5$ seconds

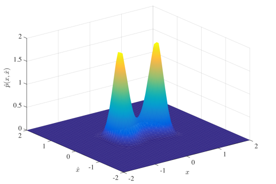


(b) $t=10$ seconds

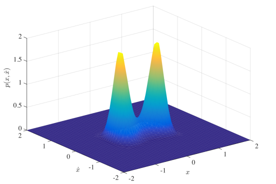


(c) $t=20$ seconds

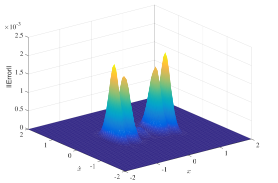
FIGURE: (3.7) Duffing Oscillator: PDF Contours



(a) Approximate Stationary PDF



(b) True Stationary PDF

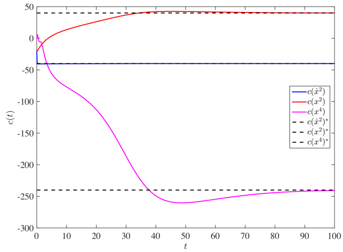


(c) Error in Stationary PDF

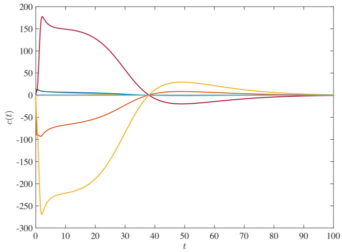
Figure: (3.9) Duffing Oscillator: Stationary PDFs

Sparse Collocation Approach

Duffing Oscillator: $\ddot{x} + \eta\dot{x} + \alpha x + \beta x^3 = g(t,x)\Gamma(t)$

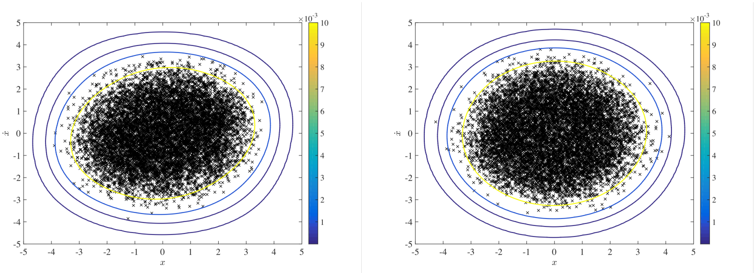


(a) Non-Zero Coefficients



(b) Zero Coefficients

FIGURE: (3.10 and 3.11) Duffing Oscillator: Coefficient Transients

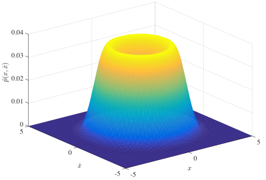


(a) $t = 2$ seconds (b) $t = 5$ seconds

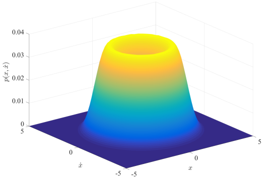
FIGURE: (3.12) Van-der-Pol Oscillator - PDF Contours

Sparse Collocation Approach

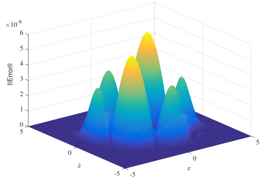
Van-der-Pol Oscillator: $\ddot{x}+\beta\dot{x}+x+\alpha(x^2+\dot{x}^2)\dot{x}=g(t,x)\Gamma(t)$



(a) Approximate Stationary PDF

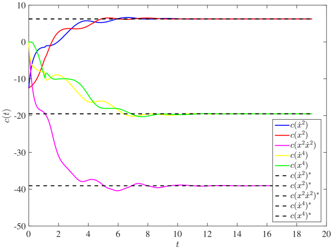


(b) True Stationary PDF

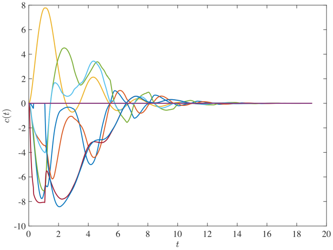


(c) Error in Stationary PDF

Figure: (3.14) Van-der-Pol Oscillator - Stationary PDFs

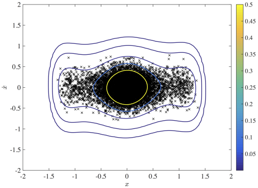


(a) Non-Zero Coefficients

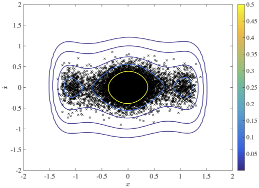


(b) Zero Coefficients

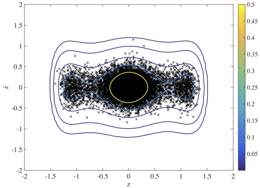
Figure: (3.15 and 3.16) Van-der-Pol - Coefficient Transients



(a) $t = 10$ seconds

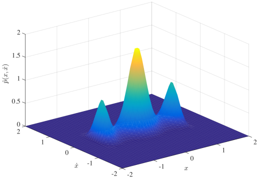


(b) $t = 20$ seconds

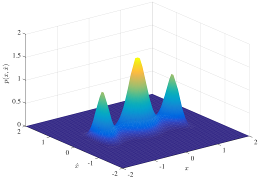


(c) $t = 30$ seconds

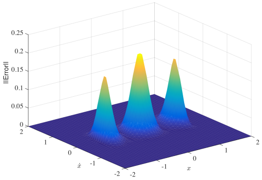
Figure: (3.17) Quintic Oscillator - PDF Contours



(a) Approximate Stationary PDF

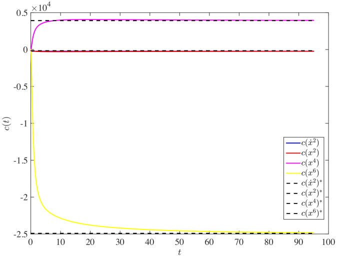


(b) True Stationary PDF

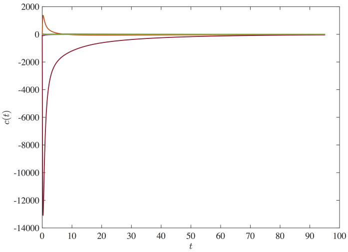


(c) Error in Stationary PDF

FIGURE: (3.19) Quintic Oscillator - Stationary PDFs



(a) Non-Zero Coefficients



(b) Zero Coefficients

FIGURE: (3.20 and 3.21) Quintic Oscillator - Coefficient Transients

- The governing dynamics are given as:

$$\ddot{\mathbf{r}} = -\frac{\mu}{r^3}\mathbf{r} + \mathbf{J}_2 \tag{13}$$

- The non-spherical gravitational perturbation is expressed as:

$$J_{2_x} = -1.5 J_2 \frac{\mu}{r^2}\left(\frac{R_e}{r}\right)^2 (1 - 5\frac{z^2}{r^2})\frac{x}{r} \tag{14}$$

$$J_{2_y} = -1.5 J_2 \frac{\mu}{r^2}\left(\frac{R_e}{r}\right)^2 (1 - 5\frac{z^2}{r^2})\frac{y}{r} \tag{15}$$

$$J_{2_z} = -1.5 J_2 \frac{\mu}{r^2}\left(\frac{R_e}{r}\right)^2 (3 - 5\frac{z^2}{r^2})\frac{z}{r} \tag{16}$$

- It is assumed that the initial state is characterized by its (known) PDF: $\mathbf{x}_0 \sim p(\mathbf{x}_0)$.

- In the absence of process noise, the FPKE reduces to Liouville's Equation:

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = -\frac{\partial p(\mathbf{x},t)}{\partial \mathbf{x}}^T \mathbf{f}(\mathbf{x},t) - p(\mathbf{x},t)\cdot Tr\left[\frac{\partial \mathbf{f}(\mathbf{x},t)}{\partial \mathbf{x}}\right] \qquad (17)$$

- Let $\mathbf{x}(t) = \phi(\mathbf{x}_0, t_0)$ be an invertible, continuously differentiable mapping, with inverse given by: $\mathbf{x}_0 = \phi^{-1}(\mathbf{x}(t), t)$.
- The *transformation of variables* (TOV) technique can be used to obtain a solution for the PDF of $\mathbf{x}(t)$ as:

$$p(\mathbf{x}(t),t) = p\left[\mathbf{x}_0 = \phi^{-1}(\mathbf{x}(t),t)\right]\left|\frac{\partial \phi^{-1}}{\partial \mathbf{x}(t)}\right| \qquad (18)$$

  - This allows for determination of the propagated PDF from knowledge of the initial PDF!

- Define the state transition matrix:

$$\Phi(t,t_0) = \frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}_0} \tag{19}$$

- Time evolution expressed as:

$$\dot{\Phi}(t,t_0) = \mathbf{A}(t)\Phi(t,t_0), \quad \mathbf{A}(t) = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{\mathbf{x}(t)} = \nabla \mathbf{f}(\mathbf{x},t) \tag{20}$$

- TOV solution can be rewritten as:

$$p(\mathbf{x}(t),t) = p\left[\mathbf{x}_0 = \phi^{-1}(\mathbf{x}(t),t)\right]\left|\Phi(t,t_0)^{-1}\right| \tag{21}$$

- Determinant evolves according to:

$$|\Phi(t,t_0)| = \exp\left(\int_0^t \nabla \cdot \mathbf{f}(\mathbf{x},s)\, ds\right) \tag{22}$$

$$\boxed{p(\mathbf{x}(t)) = p\left[\mathbf{x}_0 = \phi^{-1}(\mathbf{x}(t),t)\right]\exp\left(-\int_0^t \nabla \cdot \mathbf{f}(\mathbf{x}(s),s)ds\right)}$$

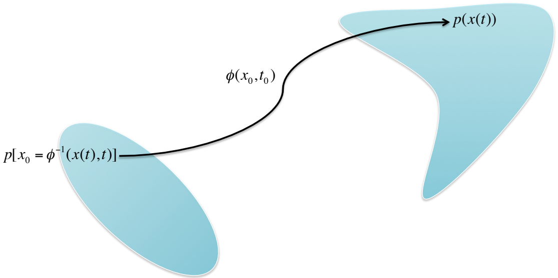


FIGURE: Evolution of Sample Probability

- Existence of the true PDF solution allows for determination of discrete probability values at any time instant!
  - Sample taken from initial PDF is propagated through dynamics.
  - Initial discrete probability value mapped to current time instant via solution of Liouville's equation.
- Exploit analytical expression to avoid direct numerical solution

- Assume a series expansion for the log-PDF:

$$\beta(\mathbf{x}(t),t) = \mathbf{c}^T(t)\Phi(\mathbf{x}) \tag{23}$$

- The behavior of the coefficients is not explicitly constrained by the FPKE.
  - The *departure* from the previous PDF is to be learned as:

$$p(\mathbf{x}(t_k),t_k) = \delta p(\mathbf{x}(t_k),t_k)p(\mathbf{x}(t_k),t_{k-1}) \tag{24}$$

  - Transforming into log-PDF form:

$$\beta(\mathbf{x}(t_k),t_k) = \delta\beta(\mathbf{x}(t_k),t_k) + \beta(\mathbf{x}(t_k),t_{k-1}) \tag{25}$$

- Applying the series approximation yields:

$$\beta(\mathbf{x}(t_k),t_k) \approx \mathbf{c}_k^T\Phi(\mathbf{x}) = \delta\mathbf{c}_k^T\Phi(\mathbf{x}(t_k)) + \mathbf{c}_{k-1}^T\Phi(\mathbf{x}(t_k)) \tag{26}$$

- Assume a series expansion for the log-PDF:

$$\beta(\mathbf{x}(t),t) = \mathbf{c}^T(t)\Phi(\mathbf{x}) \tag{27}$$

- The behavior of the coefficients is not explicitly constrained by the FPKE.
    - The *departure* from the previous PDF is to be learned as:

$$p(\mathbf{x}(t_k),t_k) = \delta p(\mathbf{x}(t_k),t_k)p(\mathbf{x}(t_k),t_{k-1}) \tag{28}$$

    - Transforming into log-PDF form:

$$\beta(\mathbf{x}(t_k),t_k) = \delta\beta(\mathbf{x}(t_k),t_k) + \beta(\mathbf{x}(t_k),t_{k-1}) \tag{29}$$

- Applying the series approximation yields:

$$\beta(\mathbf{x}(t_k),t_k) \approx \mathbf{c}_k^T\Phi(\mathbf{x}) = \delta\mathbf{c}_k^T\Phi(\mathbf{x}(t_k)) + \mathbf{c}_{k-1}^T\Phi(\mathbf{x}(t_k)) \tag{30}$$

- Assume a series expansion for the log-PDF:

$$\beta(\mathbf{x}(t),t) = \mathbf{c}^T(t)\Phi(\mathbf{x}) \tag{31}$$

- The behavior of the coefficients is not explicitly constrained by the FPKE.
  - The *departure* from the previous PDF is to be learned as:

$$p(\mathbf{x}(t_k),t_k) = \delta p(\mathbf{x}(t_k),t_k)p(\mathbf{x}(t_k),t_{k-1}) \tag{32}$$

  - Transforming into log-PDF form:

$$\beta(\mathbf{x}(t_k),t_k) = \delta\beta(\mathbf{x}(t_k),t_k) + \beta(\mathbf{x}(t_k),t_{k-1}) \tag{33}$$

- Applying the series approximation yields:

$$\beta(\mathbf{x}(t_k),t_k) \approx \mathbf{c}_k^T\Phi(\mathbf{x}) = \delta\mathbf{c}_k^T\Phi(\mathbf{x}(t_k)) + \mathbf{c}_{k-1}^T\Phi(\mathbf{x}(t_k)) \tag{34}$$

- The evolution of the discrete probability values along characteristic curves can be found exactly.
- Theoretically, an infinite number of samples would sample the true PDF exactly.
  - Random sampling should be avoided to ensure consistent results.
  - The CUT methodology can be used to generate a minimal set of samples from the initial PDF for propagation!
- A sparse optimization framework can be used to determine the departure PDF.
- The hard collocation constraint can be transformed into a soft constraint for numerical stability.
- To reduce numerical error propagation between time instances, the l_2 norm can be re-minimized over the truncated dictionary.
- For numerical stability, propagated points are mapped to a space of zero mean, identity covariance at each time instant.

- Initial sparse optimization:

$$\text{Sparse Optimization: } \min_{\delta \mathbf{c}_k} \quad ||\mathbf{K}\delta\mathbf{c}_k||_1 \tag{35}$$

$$\text{Soft Collocation: subject to: } ||\mathbf{A}\delta\mathbf{c}_k - \mathbf{B}(\mathbf{c}_{k-1})||_2 \leq \boldsymbol{\varepsilon} \tag{36}$$

- where:

$$\mathbf{A}_i = \Phi(\mathbf{x}_i(t_k))^T, \quad i = 1, 2, ..., N \tag{37}$$

$$\mathbf{B}_i(\mathbf{c}_{k-1}) = \log\left[p(\mathbf{x}_i(t_k))\right] - \Phi(\mathbf{x}_i(t_k))^T \mathbf{c}_{k-1}, \quad i = 1, 2, ..., N \tag{38}$$

- $\mathbf{x}_i(t_k)$ is the i^{th} sample propagated to time t_k, and $p(\mathbf{x}_i(t_k))$ is the discrete probability value of the sample at time t_k.
- The l_2 norm is minimized using the truncated dictionary as:

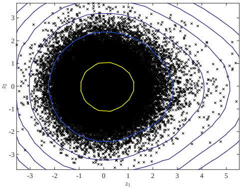
$$l_2 \text{ Conditioning: } \min_{\delta \mathbf{c}'_k} ||\mathbf{A}'\delta\mathbf{c}'_k - \mathbf{B}(\mathbf{c}_{k-1})||_2 \tag{39}$$

- The proposed method can be applied to a Sun-Synchronous Low-Earth Orbit (LEO) with initial errors characterized by:

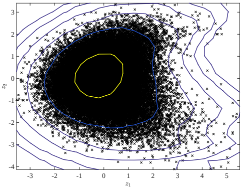
$$\boldsymbol{\mu}_0 = [7000,\ 0,\ 0,\ 0,\ -1.0374090357,\ 7.477128835]^T \quad (40)$$

$$\boldsymbol{\Sigma}_0 = diag(1, 1, 1, 1 \times 10^{-6}, 1 \times 10^{-6}, 1 \times 10^{-6}) \quad (41)$$

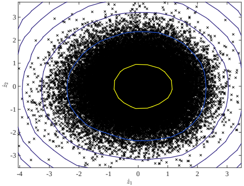
- Using CUT8-G, $N = 745$ initial conditions are available for propagation.
- Including polynomials up to eighth order results in a complete dictionary of $m = 3003$ basis functions.
- The soft constraint tolerance is chosen as $\boldsymbol{\varepsilon} = 1 \times 10^{-6}$.
- 50,000 Monte Carlo samples are available for comparison.



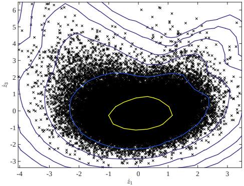
(a) (x, y) PDF Contours



(b) (x, z) PDF Contours

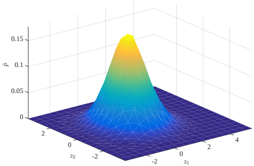


(c) $(\dot{x}, \dot{y})$ PDF Contours

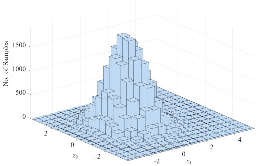


(d) $(\dot{x}, \dot{z})$ PDF Contours

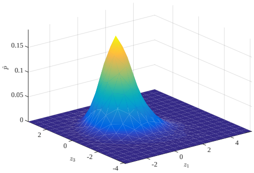
Figure: (3.22) Two-Body PDF Contours at $T/2$



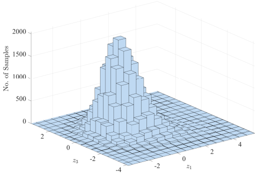
(a) (x, y) PDF Surface



(b) (x, y) Monte Carlo Hist.



(c) (x, z) PDF Surface

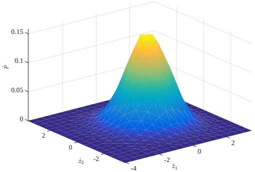


(d) (x, z) Monte Carlo Hist.

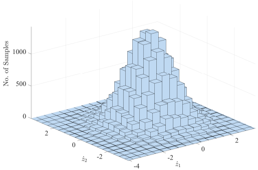
FIGURE: (3.23(a)-(d)) Posiiton PDF Surfaces and Histograms at $T/2$.

Sparse Collocation Approach

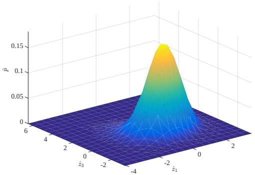
Two-Body Problem



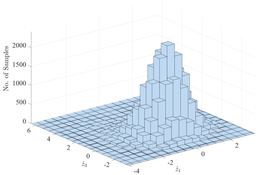
(e) $(\dot{x},\dot{y})$ PDF Surface



(f) $(\dot{x},\dot{y})$ Monte Carlo Hist.

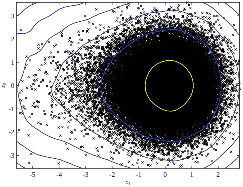


(g) $(\dot{x},\dot{z})$ PDF Surface

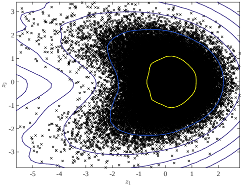


(h) $(\dot{x},\dot{z})$ Monte Carlo Hist.

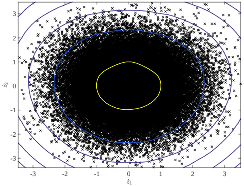
FIGURE: (3.23(e)-(h)) Velocity PDF Surfaces and Histograms at $T/2$.



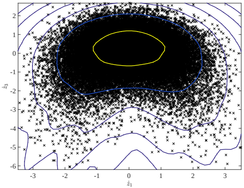
(a) (x, y) PDF Contours



(b) (x, z) PDF Contours

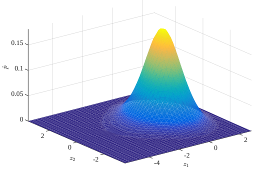


(c) $(\dot{x}, \dot{y})$ PDF Contours

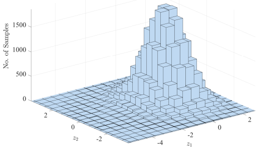


(d) $(\dot{x}, \dot{z})$ PDF Contours

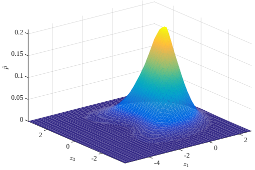
FIGURE: (3.24) Two-Body PDF Contours at T



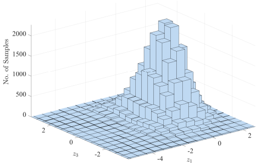
(a) (x,y) PDF Surface



(b) (x,y) Monte Carlo Hist.

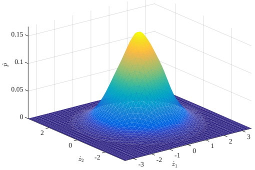


(c) (x,z) PDF Surface

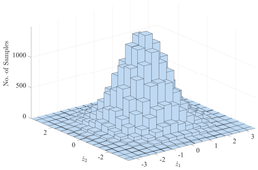


(d) (x,z) Monte Carlo Hist.

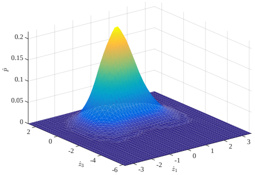
FIGURE: (3.25(a)-(d)) Posiiton PDF Surfaces and Histograms at T.



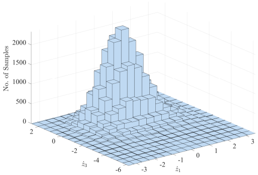
(e) $(\dot{x}, \dot{y})$ PDF Surface



(f) $(\dot{x}, \dot{y})$ Monte Carlo Hist.



(g) $(\dot{x}, \dot{z})$ PDF Surface



(h) $(\dot{x}, \dot{z})$ Monte Carlo Hist.

FIGURE: (3.25(e)-(h)) Velocity PDF Surfaces and Histograms at T.

CONCLUSIONS

- A collocation-based approach is developed to compute a solution to the Fokker-Planck-Kolmogorov Equation (FPKE).
  - The collocation points are generated using the Conjugate Unscented Transform (CUT).
  - A sparsity-enhancing l_1 optimization routine is provided to remove the non-contributing basis functions.
  - No assumptions made on structure of log-PDF!
- Numerical experiments exhibit promising results.
  - MC Histograms are well-approximated by PDF surfaces obtained.
  - Obtained PDF contours cover spread of MC points
  - For some examples, true coefficients obtained in the stationary case.
  - Stationary PDFs captured with low relative error.