Learning physics-based models from data: perspectives from inverse problems and model reduction

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Abstract

The paper *"Learning physics-based models from data: perspectives from inverse problems and model reduction"* by Ghattas and Willcox (2021) [1]presents a unified framework for learning models that are both informed by physical principles and adapted to observational data. The central focus lies in leveraging two key perspectives: inverse problems, which aim to infer unknown model parameters or states from measurements, and model reduction, which seeks to approximate complex high-dimensional systems by lower-dimensional models.

The authors emphasize the importance of exploiting the low-dimensional structure inherent in many PDE-governed physical systems. This motivates the use of projection-based techniques such as Proper Orthogonal Decomposition (POD) which is explored in-depth in this study for its ability to produce reduced-order models that retain essential physical behavior. These models serve as efficient substitutes in forward simulation and parameter estimation tasks.

In the context of inverse problems, the paper adopts a deterministic and Bayesian viewpoint, with particular attention to regularization strategies. Tikhonov regularization is examined as a classical and practical method for stabilizing ill-posed problems, particularly in high-dimensional settings with noisy data.

This work is highly relevant to the coursework, as it bridges theoretical foundations in PDE-constrained optimization with practical tools for data assimilation and reduced-order modeling. The exploration of POD, OptInf, and Tikhonov methods provides a clear and applicable pathway for solving large-scale inference problems in engineering and applied physics.

Keywords: Inverse problems, Model reduction, Proper Orthogonal Decomposition, Tikhonov regularization, Optimization-based inference

Contents

1 Introduction

The modeling of complex physical systems has traditionally relied on first-principles approaches, grounded in conservation laws and expressed through partial differential equations (PDEs). However, the rapid growth in both computational capabilities and data availability has opened new avenues for integrating observational data directly into the modeling process. This shift has sparked significant interest in methodologies that combine data with physics-based modeling, offering the potential for improved predictive accuracy, robustness to uncertainty, and computational efficiency.

In their seminal contribution, Ghattas and Willcox (2021) present a comprehensive framework for learning physics-based models from data, grounded in two complementary perspectives: inverse problems and model reduction. The authors argue that these perspectives offer a principled and scalable pathway for incorporating data into complex physical models, particularly those governed by high-dimensional PDEs. By framing the challenge as an inverse problem, one seeks to infer unknown model inputs, such as parameters, boundary conditions, or source terms, by assimilating available data. Simultaneously, model reduction techniques aim to construct low-dimensional representations of these models, significantly reducing the computational burden while preserving essential dynamical behavior.

Central to their framework is the observation that many physical systems exhibit solution manifolds that are inherently low-dimensional, despite the high dimensionality of the governing equations. This property enables the use of projection-based methods, such as proper orthogonal decomposition (POD) and Galerkin projection, to construct efficient reduced-order models (ROMs). These ROMs serve not only as surrogates for simulation but also as core components in optimization, and control.

The paper further emphasizes the scalability of the proposed methodologies. By leveraging adjoint-based techniques, randomized linear algebra, and operator-based formulations, the authors outline algorithmic strategies capable of addressing large-scale inverse problems and reduced-order modeling in practical settings. These include applications in fluid dynamics, geophysics, and other domains where PDEs serve as the foundation of physical modeling.

In summary, the work of Ghattas and Willcox provides a rigorous and unified treatment of data-driven model learning through the dual lenses of inverse problems and model reduction. It establishes a foundational framework for combining physics and data, with significant implications for scientific computing and engineering design.

2 Summary of the Review Paper

As the paper studied is a review paper, it forms a valuable scientific literature that gives an idea about the existing knowledge about data-driven physical model learning through the dual areas of inverse problems and model reduction.

The goal of the paper is to summarize the findings of existing literature about optimization-based framework for learning models that both adhere to physical laws (e.g. PDE) and are informed by observed data. The authors aim to bridge two historically separate but related fields: inverse problems (parameter estimation from observations) and model reduction (simplifying complex models for faster computation). By establishing a shared mathematical and computational language, the paper seeks to enhance the design of efficient, reliable, and scalable workflows for simulation, control in high-dimensional systems.

The paper delivers several key insights and outcomes:

- It establishes a variational formulation that unifies inverse problems and model reduction as constrained optimization problems over physical models and data.
- It emphasizes the importance of operator-centric perspectives (i.e. mapping inputs to observables or reduced coordinates), which facilitate modularity and computational scalability.
- For inverse problems, the study highlights the role of regularization and adjoint-based gradient computation as critical components of efficient large-scale inference.
- For model reduction, it shows that projection-based approaches such as Proper Orthogonal Decomposition (POD) and optimization-based inference (OptInf) can preserve physical structure while achieving substantial computational savings.

- The authors advocate for hybridization of physics and data-driven techniques, enabling models that are interpretable, generalizable, and grounded in domain knowledge.

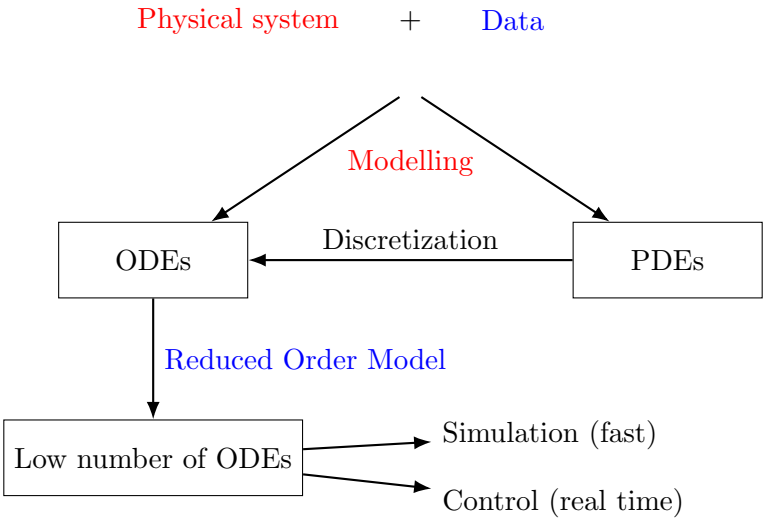
Inverse Problems

The inverse problem approach in the paper is framed as a PDE-constrained optimization problem, where the goal is to estimate unknown parameters or states that explain observed data. The key methods include:

- **Variational formulation**: Define a loss functional that balances data fidelity and regularization.
- **Tikhonov regularization**: A classical method for stabilizing ill-posed problems by penalizing undesirable parameter features.
- **Adjoint-based gradients**: Efficient computation of sensitivities in high-dimensional parameter spaces using the adjoint method.
- **Deterministic and Bayesian perspectives**: The paper discusses both point estimation and uncertainty quantification in the inverse setting.

Model Reduction

When we model a physical system, we typically start from governing equations, such as PDEs or ODEs. These are then discretized for simulation, and solving them with full resolution is computationally intensive.Model reduction happens at this stage: we aim to replace a high-dimensional system with a low-dimensional one, this is done while preserving essential system behavior, like stability or energy conservation. This is crucial for tasks requiring repeated evaluations, like control or optimization.



There are several classes of model reduction:

- Projection-Based: Use mathematical projection (e.g., Galerkin, Reduced Basis).
- Non-Intrusive: Use data-driven methods like regression or machine learning, without knowing the full model.
- Nonlinear: Use tools like manifold learning (autoencoders) to capture complex, nonlinear dynamics.

3 In-Depth Analysis of Selected Methods

3.1 Inverse Problem

The Poisson equation is a fundamental partial differential equation in physics and engineering:

$$-\nabla^2 u = m(\mathbf{x}), \quad \mathbf{x} \in \Omega \tag{3.1}$$

with boundary conditions such as:

$$u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial\Omega. \tag{3.2}$$

It appears in problems involving electrostatics, and fluid dynamics.

Example: A thin charged plate ($x \in [0, L]$) with a charge density $\rho(x)$ obeys the Poisson equation that describes the electric potential $u(\mathbf{x})$ in the presence of the charge density:

$$-\frac{d^2u}{dx^2} = \frac{\rho(x)}{\varepsilon_0}, \quad 0 < x < L. \tag{3.3}$$

where:

- $u(\mathbf{x})$ is the electric potential at position $\mathbf{x}$.
- ε_0 is the permittivity of free space.

The solution $u(\mathbf{x})$ describes how the electric potential spreads due to a given charge distribution $\rho(\mathbf{x})$.

Let's consider the following 1D poisson equation :

$$\begin{aligned} -k\frac{\partial^2 u}{\partial x^2} &= m(x) \ , \quad 0 < x < L \\ u(0) &= u(L) = 0 \end{aligned} \tag{3.4}$$

where $k > 0$ is constant.

We define the operator A as follows

$$\mathcal{A} : u \mapsto -k\frac{\partial^2 u}{\partial x^2}$$

u is the state variable. The inverse problem consists of finding $m(x)$ for a given $u(x)$, i.e. finding the parameter to observable map $\mathcal{F}$ that maps the source m to the observable u :

$$\mathcal{F}(m) = u$$

Remark 3.1. The equation (3.4) admits a unique solution $u \in H_0^1$ for all $m \in H^{-1}$, i.e. the operator $\mathcal{A}$ is bijective[1] .

The operator $\mathcal{F}$ is well-defined, and self-adjoint thanks to the self-adjointness of $\mathcal{A}$, so its eigenvalues are reals, its eigenfunctions ([6]) $v_j(x), j = 1, 2, \ldots, \infty$, are given by

$$v_j(x) = \sin\left(\frac{j\pi x}{L}\right)$$

with associated eigenvalues:

$$\lambda_j(\mathcal{F}) = \frac{1}{k}\left(\frac{L}{j\pi}\right)^2 .$$

[1]:The proof was done during the functional analysis course.

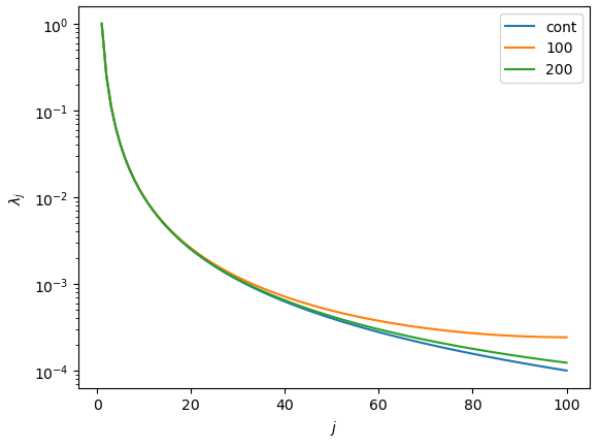


Figure 1: Spectrum of the continuous operator $\mathcal{F}$ (blue) versus that of the discretized operator $\mathcal{F}$

If $j \to \infty$, then $\lambda_j \to 0$. Thus $\mathcal{F}$ is a compact operator. Let us attempt to solve for the source $m(x)$ given $u(x)$, Then

$$\mathcal{F}(m) = u \Longrightarrow m = \mathcal{F}^{-1}u$$

Using the spectral decomposition of $\mathcal{F}$ ([6]), we obtain

$$m = \mathcal{F}^{-1}u = \sum_{j=1}^{\infty} \frac{\langle v_j, u \rangle}{\lambda_j} v_j$$

where the inner product $\langle v_j, u \rangle = \int_0^L v_j u dx$. In order for a solution m to exist, we see that the Fourier sine coefficients of the data u, $\langle v_j, u \rangle$, must decay to zero faster than the eigenvalues λ_j.

The mesured data u could contain some noise, due the instrument or its environment, model error, or numerical error in approximating $\mathcal{F}$ on the computer. We assume, in the following, that there exists additive noise η that represents the discrepancy between the data and the model output for the 'true' parameter m_{true} :

$$\mathcal{F}\left(m_{\text{true}}\right) + \eta = u$$

In this case, we can write

$$m = m_{\text{true}} + \sum_{j=1}^{\infty} \frac{\langle v_j, \eta \rangle}{\lambda_j} v_j$$

Then the error in inferring the source is given by

$$\|m - m_{\text{true}}\|^2 = \sum_{j=1}^{\infty} \frac{\eta_j^2}{\lambda_j^2}$$

where $\eta_j = \langle \nu_j, \eta \rangle$ are the Fourier components of the noise.

Since $\lambda_j^{-1} = O(j^2)$, the error grows like $O(j^2)$ in the mode number. The inference of $m(x)$ is thus unstable to small perturbations in the data. Modes v_j for which the Fourier coefficients of the noise are larger than λ_j cannot be reliably reconstructed. The inverse problem is thus ill-posed in the sense of Hadamard's instability condition.

In many inverse problems, F has a spectrum decaying to zero, making the inverse problem ill-posed (Small singular values of F amplify the noise in u, rendering direct inversion unstable). A common remedy is regularization. In the following, we will investigate the use of **Tikhonov regularization**, it consists in solving the following optimization problem:

$$\min_{m \in X} \ \phi(m) := \frac{1}{2}\|F(m) - u\|^2 + \frac{\beta}{2}\|m\|^2, \tag{3.5}$$

where $\beta > 0$ is the regularization parameter. The penalty term enforces stability by discouraging oscillatory or large-norm solutions. So it penalizes the norm of the model m, with the regularization parameter β controlling the influence of the two terms on the minimizer. Since the problem should approach the pure minimization of the data fidelity in the noise-less case it is natural to think about β as a small parameter.

This regularization parameter is chosen based on **the Morozov discrepancy principle**: select largest β^* such that

$$\|F(m_{\beta^*}) - u\| \leq \delta,$$

where δ is the noise level and m_{β^*} is the solution to the regularized problem.

⚠ In practice, we don't know the noise expression explicitly i.e. δ is unknowable.

- If the noise η is additive and normally distributed, i.e., $u = F(m_{true}) + \eta$, with $\eta \sim \mathcal{N}(0, \sigma^2 I)$, then the noise level can be estimated by

$$\delta^* \approx \sqrt{n}\,\sigma,$$

where n is the number of data points and σ is the standard deviation of the noise.

- If repeated measurements of the data are available, the noise level can be approximated by

$$\delta^* \approx \|u - \bar{u}\|,$$

where $\bar{u}$ is the empirical mean of the data across repetitions.

- If the noise is known only to satisfy $\|\eta\| \leq \delta^*$, then this bound can be directly used as the noise level in the discrepancy principle.

- If no direct information on the noise is available, one may estimate δ^* using prior knowledge of the acquisition process, instrumentation precision, or from a posteriori analysis such as residual inspection, L-curve techniques, or validation on held-out data.

In all cases, δ^* represents an estimate of the norm of the noise, and serves as a stopping criterion or tuning reference for selecting the regularization parameter β^*.

Let us show that the Morozov discrepancy principle leads to a constrained optimization problem, and that the Lagrange multiplier μ^* at the optimum is related to the regularization parameter β^* by

$$\beta^* = \frac{1}{2\mu^*}.$$

We consider the Tikhonov-regularized inverse problem:

$$m_\beta = \arg\min_{m \in X} \left(\frac{1}{2}\|F(m) - u\|^2 + \frac{\beta}{2}\|m\|^2 \right).$$

The Morozov discrepancy principle corresponds to finding the smallest penalty $\|m\|^2$ that still fits the data within the noise level[2].

This can be recast as the following constrained problem:

$$\min_{m \in X} \frac{1}{2}\|m\|^2 \quad \text{subject to } \|F(m) - u\|^2 = \delta^2.$$

To solve this, we introduce the Lagrangian:

$$\mathcal{L}(m, \mu) = \frac{1}{2}\|m\|^2 + \mu \left(\|F(m) - u\|^2 - \delta^2 \right).$$

[2]:The calculation is based on what was learned in the optimization course.

The first-order optimality condition with respect to m gives:

$$\nabla_m \mathcal{L} = m + 2\mu J_F(m)^T(F(m) - u) = 0 \Rightarrow m = -2\mu J_F(m)^T(F(m) - u),$$

where $J_F(m)$ denotes the Jacobian of F at m. On the other hand, the optimality condition for the Tikhonov problem yields:

$$J_F(m)^T(F(m) - u) + \beta m = 0.$$

Substituting the expression for m from the constrained problem into this condition leads to:

$$J_F(m)^T(F(m) - u) - 2\mu\beta J_F(m)^T(F(m) - u) = 0.$$

Thus,

$$(1 - 2\mu\beta)J_F(m)^T(F(m) - u) = 0.$$

Assuming $J_F(m)^T(F(m) - u) \neq 0$, we conclude:

$$\beta = \frac{1}{2\mu}.$$

Hence, the regularization parameter β^* chosen according to the Morozov principle is related to the Lagrange multiplier μ^* via

$$\boxed{\beta^* = \frac{1}{2\mu^*}}.$$

Solving the regularized least-squares problem offers several advantages over filter-based methods:

1. it avoids computing spectral decompositions or singular value decompositions of $\mathcal{F}$,
2. it extends to nonlinear forward operators, and allows for general norms and regularization operators [2],
3. it supports additional constraints on m such as bounds or equality conditions.

A widely used regularization is the H^1 seminorm, defined by $\int \nabla m \cdot \nabla m \, \mathrm{d}x$, which penalizes high-frequency components of m. For the model problem (3.4), its effect is to dampen the projection of m onto the eigenfunctions $v_j(x)$, with increasing weights j^2 corresponding to the eigenvalues of the 1D Laplacian associated with the H^1 seminorm.

This selectively suppresses oscillatory modes, enhancing stability.

Let's apply this to the example (3.4), using conjugate gradient to solve the optimization problem (3.5):

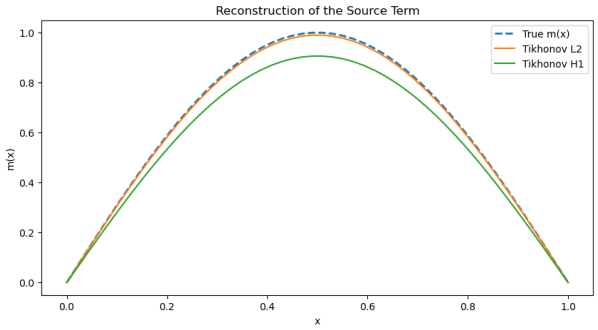


Figure 2: Recovered source term in the Poisson equation from a noisy data using Tikhonov regularization method.

3.2 Model Reduction

The model reduction framework focuses on constructing computationally efficient approximations of complex models while preserving key physical features. The techniques emphasized include:

- **Proper Orthogonal Decomposition (POD)**: A method for identifying low-dimensional bases by extracting dominant modes from simulation snapshots.
- **Galerkin projection**: Projection of governing equations onto the reduced basis to derive reduced-order models (ROMs).
- **Optimization-based inference (OptInf)**: An alternative approach that infers reduced operators from data via least-squares minimization of residuals.

These methods provide scalable alternatives to full-order simulations in tasks such as real-time prediction, control, and parameter estimation.

3.2.1 Projection-Based Method

Consider the linear PDE:

$$\frac{\partial u}{\partial t} = \mathcal{A}(u) \quad \text{in } \Omega \times (0, t_f),$$

with boundary and initial conditions, where $u(x,t) \in \mathcal{U}$ is the state at spatial location x and time t, and $\mathcal{A} : \mathcal{U} \to \mathcal{U}^*$ is the linear PDE operator.

We define the reduced model by projecting the state onto a rank r subspace $\mathcal{U}_r \subset \mathcal{U}$, spanned by orthonormal basis vectors $v_1(x), \ldots, v_r(x)$, such that:

$$u(x,t) \approx \sum_{j=1}^{r} v_j(x)\hat{u}_j(t)$$

Substituting this approximation into the governing equation gives the residual:

$$r(x,t) = \sum_{j=1}^{r} v_j \frac{\mathrm{d}\hat{u}_j}{\mathrm{d}t} - \sum_{j=1}^{r} \mathcal{A}(v_j)\hat{u}_j.$$

Galerkin projection enforces that the residual is orthogonal to the reduced space.

We will use a Galerkin projection to define the reduced model , meaning that we impose the condition : $\langle r, v_i \rangle = 0$. This yields the reduced model:

$$\frac{\mathrm{d}\hat{u}_i}{\mathrm{d}t} = \sum_{j=1}^{r} \hat{\mathcal{A}}_{ij}\hat{u}_j, \quad i = 1, \ldots, r,$$

where the reduced operator is: $\hat{\mathcal{A}}_{ij} = \langle v_i, \mathcal{A}(v_j) \rangle$, it can be precomputed once the basis is defined.

To construct the reduced basis, we use **Proper Orthogonal Decomposition** (POD): The POD basis is computed empirically from training data, typically in the form of system solutions (snapshots). It is applicable to both linear and nonlinear systems, and can be used under time-varying or parameter-varying conditions.

Let $\{s_1, s_2, \ldots, s_{n_s}\}$ be a set of n_s snapshots, where each $s_j \in \mathbb{R}^n$ denotes the j-th system state. Define the snapshot matrix $S \in \mathbb{R}^{n \times n_s}$ such that its j-th column is s_j. We aim to find an orthonormal basis $\Phi \in \mathbb{R}^{n \times r}$ such that

$$\min_{\Phi \in \mathbb{R}^{n\times r},\, \Phi^\top \Phi = I_r} \left\| S - \Phi\Phi^\top S \right\|_F^2$$

is minimized. This corresponds to minimizing the total projection error of all snapshots onto the subspace spanned by the columns of Φ.

Let S have the singular value decomposition (SVD)[3]:

$$S = U\Sigma V^\top$$

[3]:The following is done thanks to the Advanced linear algebra course.

where:

- $U \in \mathbb{R}^{n\times n}$, ($V \in \mathbb{R}^{m\times m}$), orthonormal left (right) singular vectors,
- $\Sigma \in \mathbb{R}^{n\times m}$, diagonal matrix with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, $p = \min(n, m)$.

The best rank-r approximation of S in Frobenius norm is given by the truncated SVD:

$$S_r = \sum_{i=1}^{r} \sigma_i s_i \mathbf{v}_i^\top$$

This result is guaranteed by the **Eckart-Young-Mirsky theorem**:

$$\|S - S_r\|_F = \min_{\text{rank}(B)=r} \|S - B\|_F$$

So POD basis vectors are given by the left singular vectors of S corresponding to the r largest singular values, i.e. among all r-dimensional orthonormal bases $\Phi \in \mathbb{R}^{n\times r}$ satisfying $\Phi^\top\Phi = I$, the POD basis solves:

$$\min_{\Phi\in\mathbb{R}^{n\times r},\ \Phi^\top\Phi=I} \|S - \Phi\Phi^\top S\|_F^2 = \min_{\Phi\in\mathbb{R}^{n\times r},\ \Phi^\top\Phi=I} \sum_{i=1}^{n_s} \|s_i - \Phi\Phi^\top s_i\|_2^2. \tag{3.6}$$

These vectors form an orthonormal basis $\tilde{\Phi} \in \mathbb{R}^{n\times r}$ satisfying $\tilde{\Phi}^\top\tilde{\Phi} = I$. The snapshot reconstruction error using the POD basis is given by the sum of the squares of the discarded singular values:

$$\|S - \tilde{\Phi}\tilde{\Phi}^\top S\|_F^2 = \sum_{i=1}^{n_s} \|s_i - \tilde{\Phi}\tilde{\Phi}^\top s_i\|_2^2 = \sum_{i=r+1}^{n_s} \sigma_i^2. \tag{3.7}$$

The dimension r of the POD basis is typically selected based on the decay of the singular values. **Energy Criterion:** Choose r such that:

$$\frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{n} \lambda_i} \geq \kappa \quad \text{(e.g., } \kappa = 0.99\text{)}$$

Let $\Phi = [s_1, \ldots, s_r] \in \mathbb{R}^{n\times r}$ be the matrix formed by the first r left singular vectors of S. Then the orthogonal projection of S onto the subspace spanned by Φ is:

$$\Phi\Phi^\top S = \sum_{i=1}^{r} s_i s_i^\top S = \sum_{i=1}^{r} \sigma_i s_i \mathbf{v}_i^\top = S_r$$

Hence, the projection error becomes:

$$\left\|S - \Phi\Phi^\top S\right\|_F = \|S - S_r\|_F$$

Therefore, the subspace spanned by the first r left singular vectors of the snapshot matrix S provides the optimal basis (in the sense of minimizing the Frobenius norm of the projection error). This is precisely the basis computed by the Proper Orthogonal Decomposition (POD) method.

$$\boxed{\min_{\Phi^\top \Phi = I_r} \left\| S - \Phi\Phi^\top S \right\|_F^2 = \sum_{i=r+1}^{p} \sigma_i^2}$$

Proof of the preceding:

Let $A \in \mathbb{R}^{m\times n}$ be a real matrix with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$. For any $1 \leq k < r$, the best rank-k approximation of A in the Frobenius norm is given by

$$A_k = U\Sigma_k V^T$$

where $A = U\Sigma V^T$ is the singular value decomposition (SVD) of A and Σ_k is the diagonal matrix with only the k largest singular values preserved.

Then,

$$\|A - A_k\|_F = \min_{\text{rank}(X)\leq k} \|A - X\|_F = \sqrt{\sum_{i=k+1}^{r} \sigma_i^2}.$$

Proposition 3.2.

$$\|\mathbf{A}\|_F = \left(\sum_{i=1}^{r} \sigma_i^2 \right)^{\frac{1}{2}}$$

where σ_i are the singular values of $\mathbf{A}$, and $r = \text{rank}(\mathbf{A})$.

Proof. Using the SVD $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$ we have

$$\|\mathbf{A}\|_F = \left\|\mathbf{U}^\top \mathbf{A}\right\|_F = \left\|\mathbf{U}^\top \mathbf{A}\mathbf{V}\right\|_F = \|\mathbf{\Sigma}\|_F = \text{tr}\left(\mathbf{\Sigma}^\top \mathbf{\Sigma}\right)^{\frac{1}{2}} = \left(\sum \sigma_i^2\right)^{\frac{1}{2}}$$

□

We know that any matrix can be split into the sum of rank-1 component matrices

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_i s_i \mathbf{v}_i^\top$$

We'll now consider a family of approximations of the form

$$\mathbf{A}_k = \sum_{i=1}^{k} \sigma_i s_i \mathbf{v}_i^\top$$

where $k \leq r = \text{rank}(\mathbf{A})$. This is a rank-k matrix, and as we'll now show, it is the best possible rank-k approximation to $\mathbf{A}$.

Theorem 3.3. *(Eckart-Young-Mirsky) For either the 2-norm $\|\cdot\|_2$ or the Frobenious norm $\|\cdot\|_F$, we have*

$$\|\mathbf{A} - \mathbf{A}_k\| \leq \|\mathbf{A} - \mathbf{B}\| \text{ for all rank-k matrices } \mathbf{B}.$$

Proof. **case of $\|\cdot\|_F$**

Let $A = U\Sigma V^T$ be the SVD of A, where

$$\Sigma = \begin{bmatrix} \Lambda & 0 \\ 0 & 0 \end{bmatrix}, \quad \Lambda = \text{diag}(\sigma_1, \ldots, \sigma_r),$$

with $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ orthogonal matrices.

Let X be any matrix of rank at most k, and suppose

$$X = UYV^T = U \begin{bmatrix} M & * \\ * & * \end{bmatrix} V^T,$$

where $M \in \mathbb{R}^{r\times r}$ and $\text{rank}(M) \leq k$. Then

$$\|A - X\|_F = \|U(\Sigma - Y)V^T\|_F = \|\Sigma - Y\|_F \geq \|\Lambda - M\|_F.$$

Hence, it suffices to minimize $\|\Lambda - M\|_F$ over all M of rank at most k.

Let $W \subset \mathbb{R}^r$ be the k-dimensional subspace containing the column space of M. Extend W to an orthonormal basis $\{v_1, \ldots, v_p, v_{p+1}, \ldots, v_r\}$ of $\mathbb{R}^r$, where $\{v_{p+1}, \ldots, v_r\}$ span W and $p + k = r$.

Let the columns of Λ be $(\sigma_1 e_1, \ldots, \sigma_r e_r)$ and of M be $(w_1, \ldots, w_r)$. Then

$$\|\Lambda - M\|_F^2 = \sum_{i=1}^{r} \|\sigma_i e_i - w_i\|^2.$$

To minimize this, each w_i should be the orthogonal projection of $\sigma_i e_i$ onto W:

$$\sigma_i e_i - w_i = \sum_{j=1}^{p} \langle \sigma_i e_i, v_j \rangle v_j.$$

Therefore,

$$\min \|\Lambda - M\|_F^2 = \sum_{i=1}^{r} \sum_{j=1}^{p} \langle e_i, v_j \rangle^2 \sigma_i^2.$$

The coefficients $\sum_{j=1}^{p}\langle e_i, v_j\rangle^2$ satisfy $0 \leq \sum_{j=1}^{p}\langle e_i, v_j\rangle^2 \leq 1$ and

$$\sum_{i=1}^{r}\sum_{j=1}^{p}\langle e_i, v_j\rangle^2 = p.$$

Since the σ_i^2 are in descending order, the minimum is achieved when the coefficients are concentrated on the smallest σ_i^2 (proposition 6.1), i.e.,

$$\sum_{i=1}^{r}\sum_{j=1}^{p}\langle e_i, v_j\rangle^2\sigma_i^2 \geq \sum_{i=k+1}^{r}\sigma_i^2.$$

Thus,

$$\min_{\text{rank}(X)\leq k}\|A - X\|_F^2 \geq \sum_{i=k+1}^{r}\sigma_i^2.$$

Since A_k achieves this bound, the proof is complete.

□

In what follow, we illustrate the use of Proper Orthogonal Decomposition (POD) to reduce the order of a linear dynamical system. We show that when applied to a stable system, the reduced model obtained via POD can preserve the system's stability (Section 5.2).

We consider the heat equation discretized in space:

$$\frac{dx}{dt} = Ax + Bu(t), \quad y = Cx$$

where $A \in \mathbb{R}^{n\times n}$ is the discretized Laplacian operator in 1D with Dirichlet boundary conditions. The matrices $B \in \mathbb{R}^{n\times 1}$ and $C \in \mathbb{R}^{1\times n}$ define input and output coupling at the middle of the domain.

Let $n = 100$, and the domain length $L = 1$. The matrix A is given by:

$$A = \frac{\alpha}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & & 0 \\ 1 & -2 & 1 & & \\ 0 & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 1 & -2 \end{bmatrix}$$

where $\alpha = 0.01$ is the diffusion coefficient and $\Delta x = \frac{L}{n+1}$.

The input $u(t) = \sin(2\pi t)$ is applied over time.

We simulate the FOM over the time interval $[0, 5]$ using 300 time points. The state trajectories $x(t) \in \mathbb{R}^n$ are collected into a snapshot matrix $X \in \mathbb{R}^{n \times m}$.

We then apply the Singular Value Decomposition (SVD):

$$X = U\Sigma V^T$$

and retain the first $r = 3$ columns of U, denoted U_r, as the reduced basis. The reduced-order model (ROM) is then defined by:

$$\frac{dz}{dt} = A_r z + B_r u(t), \quad y_r = C_r z$$

with

$$A_r = U_r^T A U_r, \quad B_r = U_r^T B, \quad C_r = C U_r$$

Figure 3 shows the time response of the full-order model and the reduced-order model.

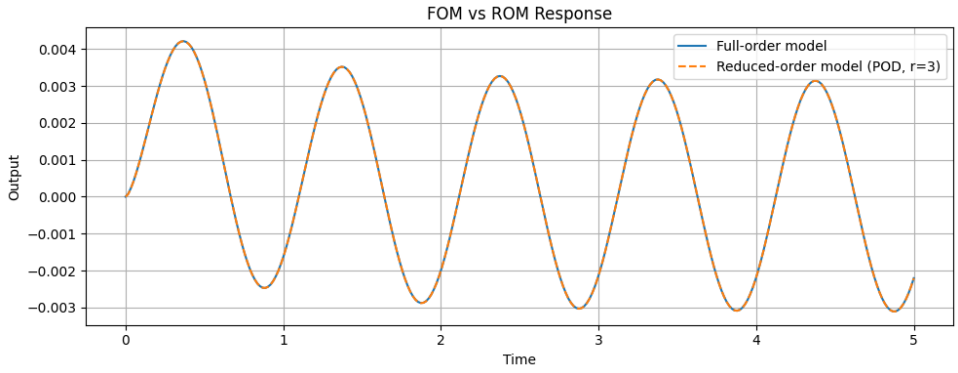


Figure 3: Output response of the full-order model (FOM) and reduced-order model (ROM) using POD (r = 3).

We also compute the eigenvalues of both A and A_r. Table 1 shows the maximum real part of the eigenvalues in both models.

Model	Max Real Part of Eigenvalues	Execution time
Full-order (FOM)	$-0.9869403481356569 < 0$	29.401416301727295
Reduced-order (ROM)	$-0.9920437792538935 < 0$	0.03446221351623535

Table 1: Comparison of stability (all poles in left half-plane), and time of the programs' execution.

Remark 3.4. The results depends on the number n_s of snapshots.

We can alsoshow that model order reduction helps for faster simulations 1:

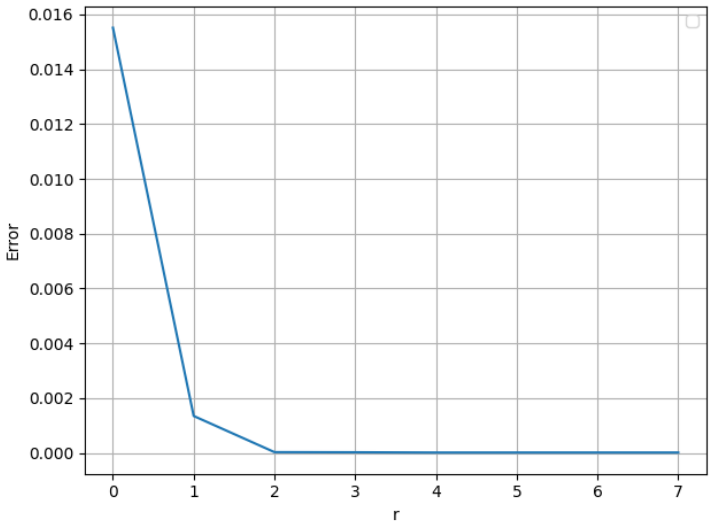


Figure 4: $\|y_{fom} - y_{rom}\|_2$ as function of r

4 Discussion and Critical Analysis

The review by Ghattas and Willcox presents a compelling and structured synthesis of two major paradigms in mathematical modeling: inverse problems and model reduction. A key strength of the paper lies in its conceptual clarity and unified treatment of these fields, offering a coherent framework for combining physics-based models with observational data. The authors' emphasis on physical consistency, computational scalability, and algorithmic modularity renders the approach particularly suitable for large-scale systems governed by PDEs.

Another notable strength is the scalability of the proposed methods. The discussion of projection-based model reduction, particularly via POD and OptInf, is grounded in practical algorithmic considerations. The framework accommodates adjoint-based gradient computations, randomized linear algebra, and operator inference, enabling real-world applicability to complex systems such as fluid flow, structural mechanics, and subsurface modeling.

Furthermore, the paper stands out in its ability to bridge theory and practice. By contextualizing inverse problems and reduced-order modeling within a shared optimization-based paradigm, it offers a language that can support diverse applications—from control and design to uncertainty quantification.

The framework relies on several key assumptions that impact its applicability and

generalization. First, it presumes the existence of a low-dimensional manifold underlying the solution space of the governing PDEs. This assumption is well-justified in many parametric settings but may fail in the presence of strong nonlinearities, turbulence, or high-dimensional input spaces, where the solution manifold is highly non-smooth.

Second, the inverse problem formulation typically assumes additive Gaussian noise in the data and smooth parameter-to-observable maps. While these assumptions simplify the theoretical and computational treatment, they may not hold in real-world applications involving non-Gaussian noise, outliers, or discontinuities. Moreover, the reliance on Tikhonov regularization implies a preference for smooth solutions, potentially suppressing sharp features or discontinuities that may be physically meaningful.

Third, the projection-based ROMs assume that the system dynamics can be faithfully represented in a fixed low-dimensional subspace. This can be problematic in time-varying or multi-regime systems, where a static reduced basis may be insufficient to capture transient dynamics or switching behaviors, and the Greedy algorithm introduced in the paper, to solve such a problems, is not treated from a convergence point.

Despite its elegance, the proposed framework faces several limitations. Most notably, the scalability of reduced-order models in the presence of nonlinearity remains a significant challenge. While the authors touch upon operator inference and nonlinear Galerkin projection, the practical deployment of ROMs in highly nonlinear systems is still limited. Future work could explore localized or adaptive basis methods, hyper-reduction techniques, or nonlinear manifold learning as potential remedies.

In the inverse problem context, the use of classical regularization techniques such as Tikhonov is well-motivated but may lack robustness when dealing with sparse or unstructured data. Alternative approaches, such as total variation regularization, or iteratives methods using Bregman [2], could offer better fidelity in reconstructing complex or discontinuous parameter fields.

Furthermore, while the paper emphasizes projection-based methods, it largely omits recent advances in machine learning–enhanced model reduction. Methods such as physics-informed neural networks (PINNs), deep autoencoders for reduced latent representations, and neural operator learning could be integrated into the proposed framework to improve adaptability and generalization to unseen inputs.

The conceptual clarity and methodological rigor of this paper make it a foundational reference in the intersection of physics-based modeling and data-driven inference.

The operator-centric perspective, in particular, has inspired subsequent work on data-driven discovery of dynamical systems, learning PDE operators from data, and hybrid methods that blend first-principles models with data-driven corrections. The emphasis on adjoint-based optimization and scalable solvers has also helped bridge high-performance computing and uncertainty quantification communities.

In summary, the paper presents a robust and versatile framework for integrating data and physics in large-scale modeling. Its strengths lie in theoretical unification, algorithmic scalability, and broad applicability. However, its applicability could be limited in some problems. Addressing these challenges will require the integration of more flexible learning architectures, adaptive model reduction techniques, and robust inverse problem formulations.

5 Future Directions and Open Questions

5.1 Model reduction of Port-Hamiltonian systems

We consider a finite-dimensional pH system of the form

$$\begin{cases} \dot{\mathbf{x}}(t) = (\mathbf{J} - \mathbf{R})\nabla_{\mathbf{x}} H(\mathbf{x}(t)) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{B}^\top \nabla_{\mathbf{x}} H(\mathbf{x}(t)) \end{cases} \tag{5.1}$$

with $\mathbf{x}(0) = \mathbf{x}^0$, where $\mathbf{x}(t) \in \mathbb{R}^n$ represents the n-dimensional state vector, $H(\mathbf{x})$ is the Hamiltonian function, which is continuously differentiable and represents the internal energy of the system, the matrix $\mathbf{J} = -\mathbf{J}^\top \in \mathbb{R}^{n\times n}$ is skew-symmetric, describing the interconnection of the system's energy storage elements; the matrix $\mathbf{R} = \mathbf{R}^\top \in \mathbb{R}^{n\times n}$ is symmetric and positive semi-definite, characterizing the energy dissipation in the system, $\mathbf{B} \in \mathbb{R}^{n\times m}$ is the port matrix, which describes the modalities through which energy is imported into or exported from the system, $\mathbf{u}(t) \in \mathbb{R}^m$ represents the external input vector, and $\mathbf{y}(t) \in \mathbb{R}^m$ is the system's output vector. Based on the structural properties of $\mathbf{J}$ and $\mathbf{R}$, one can conclude that the Hamiltonian function satisfies the dissipation inequality:

$$\begin{aligned}\frac{dH}{dt}(\mathbf{x}(t)) &= \nabla_{\mathbf{x}} H(\mathbf{x}(t))^{\top}.\frac{dx}{dt} \\ &= \left(\nabla_{\mathbf{x}} H(\mathbf{x}(t))^{\top}\left[(\mathbf{J}-\mathbf{R})\nabla_{\mathbf{x}} H(\mathbf{x}(t)+\mathbf{B}\mathbf{u}(t)\right]\right) \\ &\leq \mathbf{y}(t)^{\top}\mathbf{u}(t)\end{aligned} \tag{5.2}$$

We seek a reduced-order model via a Galerkin projection using a basis $V \in \mathbb{R}^{n\times r}$ with orthonormal columns. The reduced state is $\hat{x} \in \mathbb{R}^r$, and the full state is approximated as $x \approx V\hat{x}$.

We define the reduced Hamiltonian as the restriction of the full Hamiltonian to the reduced subspace:

$$\hat{H}(\hat{x}) := H(V\hat{x}).$$

Although $V\hat{x} \in \mathbb{R}^n$, the function $\hat{H}$ depends only on the reduced variable $\hat{x} \in \mathbb{R}^r$, and thus qualifies as a reduced Hamiltonian. We have then

$$\nabla_{\hat{x}}\hat{H}(\hat{x}) = V^{\top}\nabla_x H(V\hat{x})$$

Using Galerkin projection, the reduced dynamics are:

$$\begin{aligned}\frac{d\hat{x}}{dt} &= V^{\top}\dot{x}(t) \\ &= V^{\top}[(J-R)\nabla_x H(V\hat{x}) + Bu(t)] \\ &= V^{\top}[(J-R)VV^{\top}\nabla_x H(V\hat{x}) + Bu(t)] \\ &= (V^{\top}JV - V^{\top}RV)\nabla_{\hat{x}}\hat{H}(\hat{x}) + V^{\top}Bu(t).\end{aligned}$$

One identifies the reduced-order operators as:

$$J_r = V^{\top}JV,\ R_r = V^{\top}RV, \text{ and } B_r = V^{\top}B.$$

We obtain a structure-preserving Galerkin projection-based for the pH system (5.1) as

$$\begin{cases}\dot{\hat{x}}(t) = (\mathbf{J}_r - \mathbf{R}_r)\,\nabla_{\hat{x}}\hat{H}\,(\hat{x}(t)) + \mathbf{B}_r\mathbf{u}(t), \\ \mathbf{y}_r(t) = \mathbf{B}_r^{\top}\nabla_{\hat{x}}\hat{H}\,(\hat{x}(t))\end{cases}$$

with the initial condition

$$\hat{x}(0) = V^{\top}\mathbf{x}^0$$

Due to the same structure as its full-order counterpart, the time derivative of the reduced Hamiltonian is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{H}\left(\hat{x}(t)\right) &= \nabla_{\hat{x}}\hat{H}\left(\hat{x}(t)\right)^{\top}.\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} \\ &= \nabla_{\hat{x}}\hat{H}\left(\hat{x}(t)\right)^{\top}\left[(J_r - R_r)\nabla_{\hat{x}}\hat{H}\left(\hat{x}(t)\right) + B_r\mathbf{u}(t)\right] \\ &\leq \nabla_{\hat{x}}\hat{H}\left(\hat{x}(t)\right)^{\top} B_r\mathbf{u}(t) \quad \left(\text{ as } J_r = -J_r^{\top}, R_r = R_r^{\top} \text{ and } R_r \succcurlyeq \mathbf{0}\right) \\ &= \mathbf{y}_r(t)^{\top}\mathbf{u}(t)\end{aligned}$$

therefore, the dissipation inequality (5.2) holds at the reduced-order level.

5.2 Stability Preservation under Galerkin Projection

Consider the linear time-invariant (LTI) dynamical system:

$$\frac{dx}{dt} = Ax, \quad x(0) = x_0 \in \mathbb{R}^n,$$

where $A \in \mathbb{R}^{n\times n}$ is a constant matrix, such that A is Hurwitz, i.e., all eigenvalues of A have strictly negative real parts.

Let $V \in \mathbb{R}^{n\times r}$ be a matrix with orthonormal columns, i.e., $V^{\top}V = I_r$. We define the approximation to the full state as $x(t) \approx V\hat{x}(t)$. The Galerkin reduced-order model is:

$$\frac{d\hat{x}}{dt} = \hat{A}\hat{x}, \quad \text{with } \hat{A} = V^{\top}AV, \quad \hat{x}(0) = V^{\top}x_0.$$

Since A is Hurwitz, there exists a symmetric positive definite matrix $P \in \mathbb{R}^{n\times n}$ such that:

$$A^{\top}P + PA = -Q, \quad \text{for any } Q = Q^{\top} > 0.$$

Let $\hat{P} = V^{\top}PV$ and $\hat{Q} = V^{\top}QV$. Then $\hat{P}$ is symmetric positive definite since:

$$\hat{x}^{\top}\hat{P}\hat{x} = (V\hat{x})^{\top}P(V\hat{x}) > 0 \quad \forall \hat{x} \neq 0,$$

because $P > 0$ and $V\hat{x} \neq 0$ if $\hat{x} \neq 0$.

Compute:

$$\hat{A}^{\top}\hat{P}+\hat{P}\hat{A} = (V^{\top}AV)^{\top}(V^{\top}PV)+(V^{\top}PV)(V^{\top}AV) = V^{\top}(A^{\top}P+PA)V = -V^{\top}QV = -\hat{Q}.$$

Since $\hat{Q} > 0$, $\hat{A}$ is Hurwitz and the reduced system is asymptotically stable.

The reduced-order model obtained via Galerkin projection preserves the asymptotic stability of the full-order system. This follows directly from the existence of a Lyapunov function for the FOM and its projection to the reduced subspace.

5.3 Application of model reduction to solving inverse problems

In many applications, inverse problems arising from partial differential equations may be ill-posed in the sense that the solutions may not depend continuously on the data. Such issues severely impact the stability and reliability of numerical reconstructions. To mitigate this, one may consider constructing ROMs that approximate the original high-dimensional system while preserving its essential dynamics. Given that the inverse problem is ill-posed, a natural question arises: can one construct a reduced-order model of the system with the aim of obtaining a well-posed reduced inverse problem?

6 Conclusion

The integration of physics-based modeling with data-driven inference represents a transformative direction in computational science. The framework developed by Ghattas and Willcox demonstrates how inverse problems and model reduction can be employed to construct efficient and accurate models that assimilate data while respecting the underlying physics. Their approach is particularly compelling in settings governed by high-dimensional PDEs, where both computational cost and uncertainty present significant challenges.

Looking ahead, several promising directions emerge from this foundational work. One avenue for future research is the extension of model reduction techniques to strongly nonlinear or parametric systems, where classical projection-based methods may struggle. Additionally, there is growing interest in hybrid approaches that integrate machine learning techniques, such as neural networks or operator learning with physics-informed priors, enabling more flexible and expressive models.

Another area of ongoing development involves the treatment of uncertainty, particularly in Bayesian inverse problems. Scalable and robust algorithms for high-dimensional posterior inference remain an active topic, with potential benefits for risk quantification and decision-making in complex systems.

In conclusion, the synthesis of inverse problem theory and model reduction offers a powerful paradigm for learning from data in physics-based settings, as computational tools and data sources continue to evolve.

Continued development along these lines, especially at the interface of scientific machine learning and physics-based inference, holds great promise for improving the efficiency and reliability of predictive models in complex and high-dimensional systems.

Appendix

Proposition 6.1. ***Extreme Point Optimality:*** *Let $C \subseteq \mathbb{R}^n$ be a nonempty polyhedron, and let $f(x) = c^T x$ be a linear function. If x^* minimizes $f(x)$ over C, then there exists an extreme point $\bar{x} \in C$ such that $f(\bar{x}) = f(x^*)$.*

Proof. Let $C = \{x \in \mathbb{R}^n \mid Ax \leq b\}$ be a nonempty polyhedron, and assume $x^* \in C$ is a minimizer of the linear function $f(x) = c^T x$ over C.

Polyhedra are convex sets. By definition, polyhedra are convex. That means for any two points $x_1, x_2 \in C$, the line segment between them is also in C.

Convex sets are the convex hull of their extreme points. From convex geometry (specifically, the Minkowski-Weyl theorem), every bounded polyhedron (or any compact convex polytope) is the convex hull of its extreme points. Therefore, we can write:

$$x^* = \sum_{i=1}^{k} \lambda_i x^{(i)},$$

where $x^{(i)} \in C$ are extreme points and $\lambda_i \geq 0$, $\sum_i \lambda_i = 1$.

Linearity preserves convex combinations. Since $f(x) = c^T x$ is linear, we have:

$$f(x^*) = f\left(\sum_{i=1}^{k} \lambda_i x^{(i)}\right) = \sum_{i=1}^{k} \lambda_i f(x^{(i)}).$$

So $f(x^*)$ is a convex combination of the values $f(x^{(i)})$. If x^* is optimal, then:

$$f(x^{(i)}) \geq f(x^*) \quad \text{for all } i,$$

but since equality holds in the convex combination, we must have:

$$f(x^{(i)}) = f(x^*) \quad \text{for all } i \text{ such that } \lambda_i > 0.$$

At least one extreme point $x^{(i)}$ with $\lambda_i > 0$ satisfies $f(x^{(i)}) = f(x^*)$. Therefore, the minimum is attained at an extreme point. □

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