Regression

Purdue ME 597, Distributed Energy Resources

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Outline

What is machine learning?

- extracting information from data, usually to make predictions
- includes two general tasks:
  1. build a **model** from data
  2. **validate** the model (assess performance on **unseen** data)
- a **supervised** learning model predicts **targets** given **features**
  - ◇ **regression** predicts real-valued targets
  - ◇ **classification** predicts targets from finite sets such as $\{-1, 1\}$
- **unsupervised** learning creates a model of the data

Training and validation

- our true goal is to predict unseen data
- good practice: divide the full dataset into
  1. **training** data for choosing model **parameters**
  2. **validation** data for evaluating candidate models
- **overfit** models
  - ◇ perform well on training data, but not on validation data
  - ◇ likely won't **generalize** well to unseen data

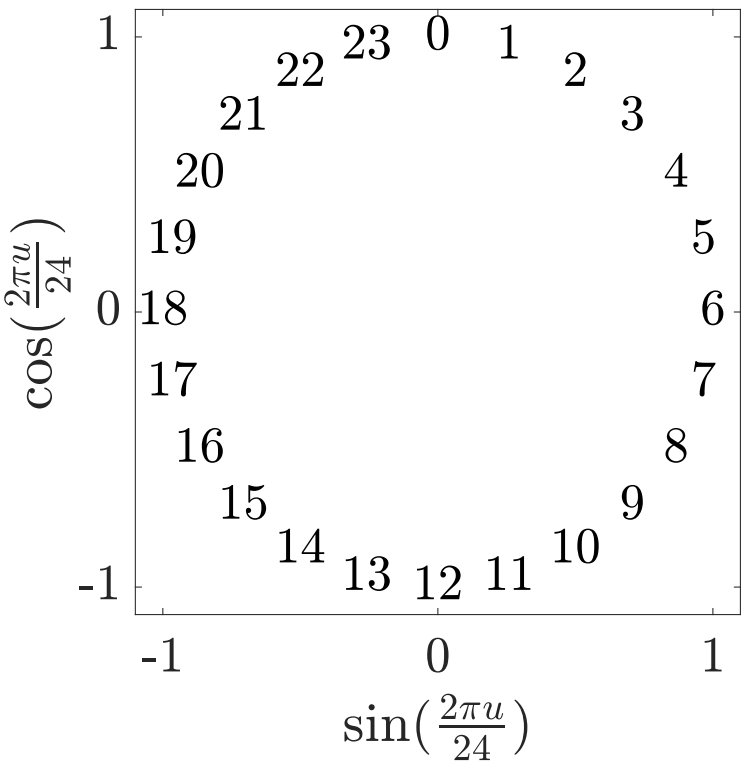
Embeddings

- denote raw input, output data by $u^{(i)} \in \mathcal{U}$, $v^{(i)} \in \mathcal{V}$
  - $\mathcal{U}$ is the set of possible input data
  - $\mathcal{V}$ is the set of possible output data
- we often transform each
  - raw input $u^{(i)}$ into a feature $x^{(i)} = \phi(u^{(i)}) \in \mathbf{R}^{n_x}$
  - raw output $v^{(i)}$ into a target $y^{(i)} = \psi(v^{(i)}) \in \mathbf{R}^{n_y}$
- $\phi : \mathcal{U} \to \mathbf{R}^{n_x}$ and $\psi : \mathcal{V} \to \mathbf{R}^{n_y}$ are called **embeddings**
- we'll assume $n_y = 1$ from now on, but methods extend to vector $y^{(i)}$

Faithful embeddings satisfy $\phi(u) \approx \phi(\tilde{u}) \iff u \approx \tilde{u}$

example: suppose $\mathcal{U} = \{0, \ldots, 23\}$ contains hour-of-day data

- problem: midnight $\approx$ 11 PM, but $0 \not\approx 23$
- idea: choose $\phi(u) = \sin(\frac{2\pi u}{24})$, so $\phi(0) \approx \phi(23)$
- new problem: midnight $\not\approx$ noon, but $\sin(0) = \sin(\pi)$
- faithful embedding: $\phi(u) = \left(\sin(\frac{2\pi u}{24}), \cos(\frac{2\pi u}{24})\right)$



Standardization and normalization

- model training tends to work better when feature scales are similar
- **standardization** and **normalization** are two ways to rescale data
- standardization embedding, $x_j^{(i)} = (u_j^{(i)} - \mu_j)/\sigma_j$ with

$$\mu_j = \frac{1}{n}\sum_{i=1}^{n} u_j^{(i)}, \ \sigma_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(u_j^{(i)} - \mu_j)^2},$$

  makes $\frac{1}{n}\sum_{i=1}^{n} x_j^{(i)} = 0$, $\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_j^{(i)})^2} = 1$

- normalization embedding, $x_j^{(i)} = (u_j^{(i)} - \underline{u}_j)/(\overline{u}_j - \underline{u}_j)$ with

$$\underline{u}_j = \min\left\{u_j^{(1)}, \ldots, u_j^{(n)}\right\}, \ \overline{u}_j = \max\left\{u_j^{(1)}, \ldots, u_j^{(n)}\right\},$$

  makes each $x_j^{(i)}$ lie between zero and one

Models

- a model is a function $f_\theta : \mathbf{R}^{n_x} \to \mathbf{R}$
- notation f_θ emphasizes dependence on parameters $\theta \in \mathbf{R}^{n_\theta}$
- a good model predicts $f_\theta(x) \approx y$ for unseen (x, y) data
- many possible model structures:
  - ◇ linear models
  - ◇ nearest neighbors
  - ◇ neural networks
  - ◇ regression trees
  - ◇ support vector machines
  - ◇ ...

Linear models

- **linear** models have the form $f_\theta(x) = \theta^\top x$ (so $n_\theta = n_x$)
- usually, we embed with a constant feature $x_1 = 1$, so

$$f_\theta(x) = \theta_1 + \theta_2 x_2 + \cdots + \theta_{n_x} x_{n_x}$$

- in training, we choose θ such that each $f_\theta(x^{(i)}) \approx y^{(i)}$:

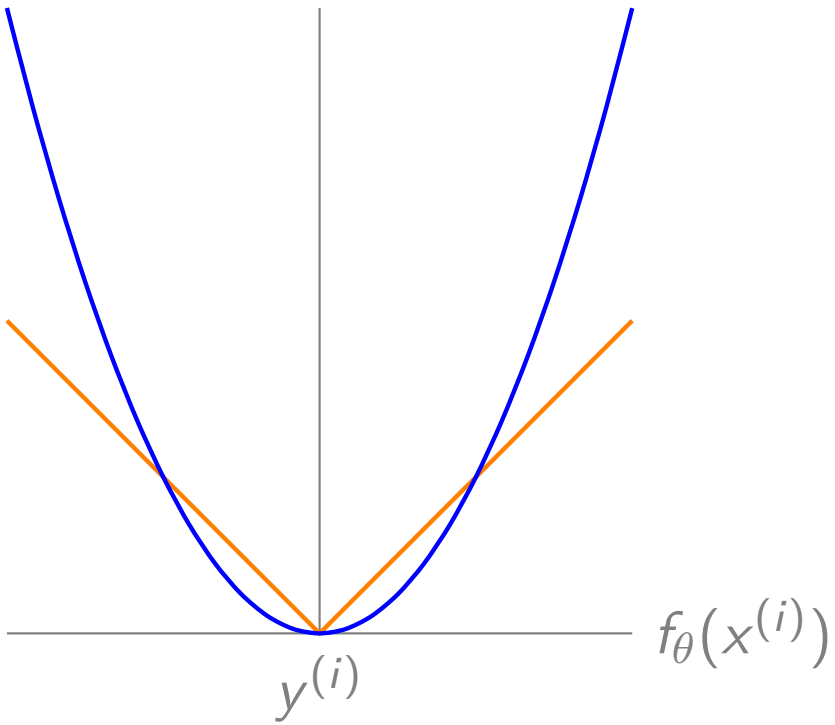
$$\begin{bmatrix} \theta^\top x^{(1)} \\ \vdots \\ \theta^\top x^{(n)} \end{bmatrix} = \begin{bmatrix} (x^{(1)})^\top \theta \\ \vdots \\ (x^{(n)})^\top \theta \end{bmatrix} = \begin{bmatrix} (x^{(1)})^\top \\ \vdots \\ (x^{(n)})^\top \end{bmatrix} \theta \approx \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

- can write this as $X\theta \approx Y$, where

$$X = \begin{bmatrix} (x^{(1)})^\top \\ \vdots \\ (x^{(n)})^\top \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & \cdots & x_{n_x}^{(1)} \\ \vdots & & \vdots \\ x_1^{(n)} & \cdots & x_{n_x}^{(n)} \end{bmatrix}, \quad Y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

Loss functions

- a loss function $\ell_i : \mathbf{R}^{n_\theta} \to \mathbf{R}$ quantifies how badly $f_\theta(x^{(i)})$ misses $y^{(i)}$
- square loss: $\ell_i(\theta) = (f_\theta(x^{(i)}) - y^{(i)})^2$
- absolute loss: $\ell_i(\theta) = \left|f_\theta(x^{(i)}) - y^{(i)}\right|$



Mean loss

- the **mean loss** $\mathcal{L} : \mathbf{R}^{n_\theta} \to \mathbf{R}$ is

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell_i(\theta)$$

- with square loss, $\mathcal{L}$ is the mean square error (MSE):

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} (f_\theta(x^{(i)}) - y^{(i)})^2$$

- with absolute loss, $\mathcal{L}$ is the mean absolute error (MAE):

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left| f_\theta(x^{(i)}) - y^{(i)} \right|$$

Regularization

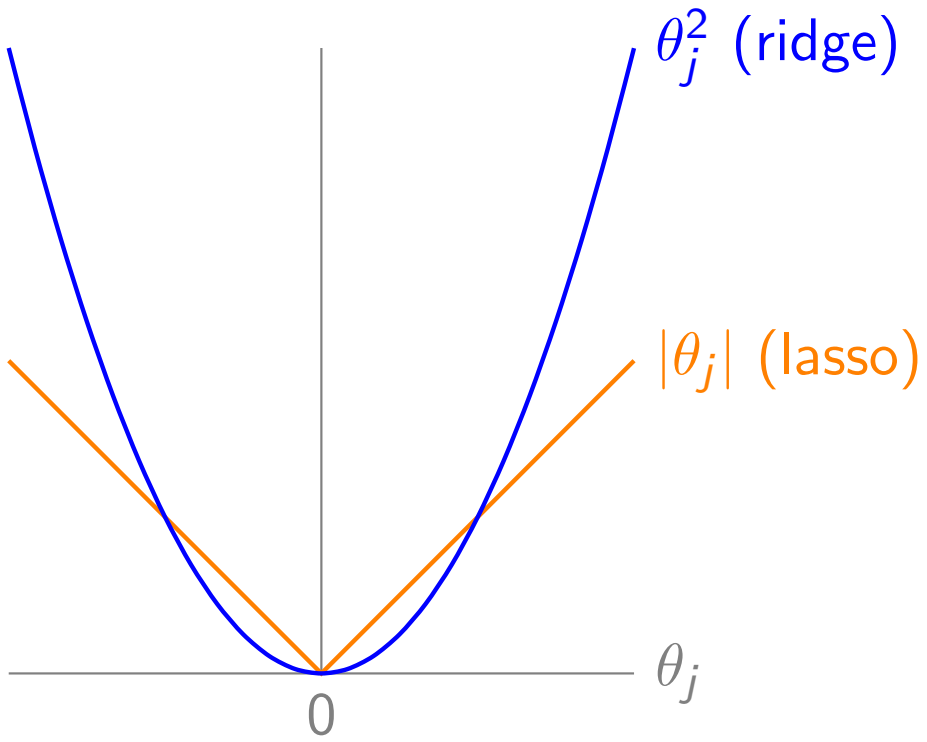
- a model f_θ is **insensitive** if $f_\theta(x) \approx f_\theta(\tilde{x})$ when $x \approx \tilde{x}$
- insensitive models tend to generalize better
- a **regularizer** $r : \mathbf{R}^{n_\theta} \to \mathbf{R}$ quantifies the sensitivity of f_θ
- for linear model $f_\theta(x) = \theta^\top x$,

$$\frac{\partial f_\theta(x)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\theta_1 x_1 + \cdots + \theta_j x_j + \cdots + \theta_{n_x} x_{n_x}\right) = \theta_j$$

  $\implies$ f_θ should be less sensitive if θ is smaller
- two common regularizers:
  - ◇ **ridge** or ℓ_2: $r(\theta) = \|\theta\|_2^2 = \theta_1^2 + \cdots + \theta_{n_\theta}^2$
  - ◇ **lasso** or ℓ_1: $r(\theta) = \|\theta\|_1 = |\theta_1| + \cdots + |\theta_{n_\theta}|$
- with constant feature $x_1 = 1$, typically omit θ_1 from regularization

Lasso regularization promotes sparsity

- a vector is **sparse** if it has few nonzero elements
- if $\theta_j = 0$ in linear model $f_\theta(x) = \theta_1 x_1 + \cdots + \theta_{n_x} x_{n_x}$, then
  - ◇ feature x_j has no influence on predictions
  - ◇ might as well omit x_j and simplify model training, evaluation
- lasso regularizer $|\theta_1| + \cdots + |\theta_{n_x}|$ promotes sparsity of θ



Training models via regularized mean loss minimization

- choosing θ is called **training** the model
- two competing goals:
  1. fit training data well by making $\mathcal{L}(\theta)$ small
  2. generalize well by making $r(\theta)$ small
- to balance them, choose θ to minimize $\mathcal{L}(\theta) + \lambda r(\theta)$
- regularization **hyperparameter** $\lambda \geq 0$ governs tradeoff: 1 vs. 2

Training linear models, $f_\theta(x) = \theta^\top x$

- with linear model, square loss, and ℓ_2 regularization,

$$\begin{aligned}\mathcal{L}(\theta) + \lambda r(\theta) &= (X\theta - Y)^\top (X\theta - Y)/n + \lambda \theta^\top \theta \\ &= (\theta^\top X^\top X\theta - 2Y^\top X\theta + Y^\top Y)/n + \lambda \theta^\top I\theta \\ &= [\theta^\top (X^\top X + n\lambda I)\theta - 2Y^\top X\theta - Y^\top Y]/n\end{aligned}$$

- since $\mathcal{L}(\theta) + \lambda r(\theta) = \theta^\top P\theta + q^\top \theta + r$, gradient is $2P\theta + q$

$$2P\theta^\star + q = 0 \iff \theta^\star = (X^\top X + n\lambda I)^{-1} X^\top Y$$

- inverse always exists if $\lambda > 0$
- if $\lambda = 0$ (no regularization), X needs linearly independent columns
- to omit θ_1 regularization, replace I_{n_x} by $E^\top E$, where

$$E = \begin{bmatrix} 0 & I_{n_x - 1} \end{bmatrix} \in \mathbf{R}^{n_x - 1 \times n_x}$$

- no formula for absolute loss or ℓ_1 regularization, but convex problems

Validation

- true goal: choose embeddings ϕ, ψ and model f_θ such that

$$\psi^{-1}(f_\theta(\phi(u))) \approx v$$

  for unseen (u, v) data
- we can't test this until unseen data are revealed
- instead, validation
  - ◇ holds back some data from training
  - ◇ evaluates performance on held-back data

Out-of-sample validation

- split data into training and validation (say, 70/30, 80/20, or 90/10)
- choose starter embeddings, model structure, hyperparameters
- repeat:
  - ◇ change embeddings, model structure, or hyperparameters
  - ◇ train model in training data
  - ◇ if performance degrades in validation data, revert change

  until performance in validation data is acceptable

K-folds validation

- divide data into K **folds**
- for $k = 1, \ldots, K$
  - ◇ train on all data except fold k
  - ◇ compute mean loss on fold k, $\mathcal{L}_k(\theta)$
- evaluate performance using mean (over all folds) of mean losses,

$$\bar{\mathcal{L}}(\theta) = \frac{1}{K} \sum_{i=1}^{K} \mathcal{L}_k(\theta)$$

Summary: How to build regression models

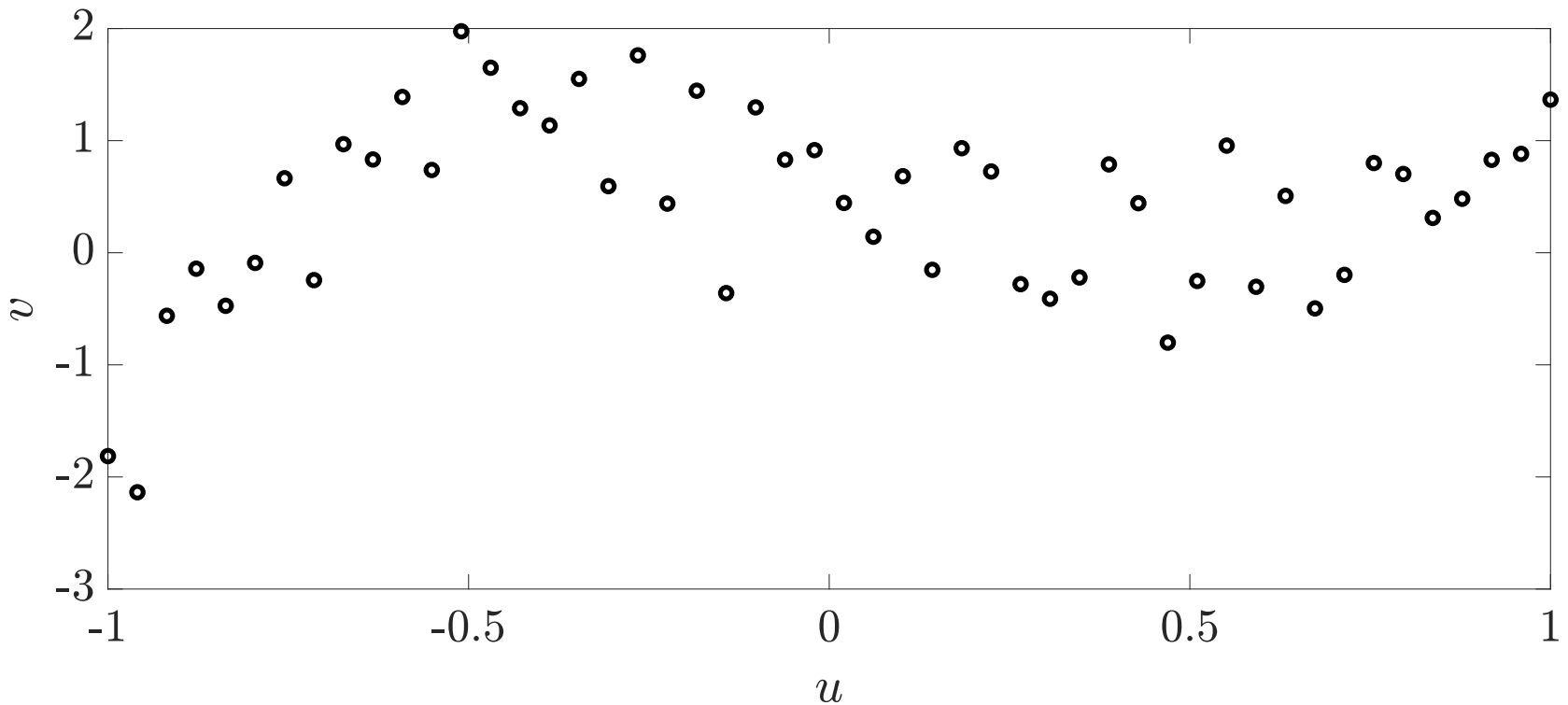
- choose a loss function to rate how badly predictions miss targets
- choose a regularizer to rate model sensitivity
- split data into training and validation
- repeat:
  - ◇ choose how to embed raw data into features and targets (**feature engineering**)
  - ◇ choose a model structure and hyperparameters (**model selection** and **hyperparameter tuning**)
  - ◇ choose model parameters to minimize regularized mean training loss (**training**)

  until validation performance is acceptable
- retrain model on all (training + validation) data

Outline

Problem

- goal: approximate an unknown function $g : [-1, 1] \to \mathbf{R}$
- $n = 50$ noisy raw data points:
  - ◇ inputs $u^{(1)}, \ldots, u^{(50)}$ are evenly spaced on $[-1, 1]$
  - ◇ outputs $v^{(i)}$ are noisy observations of $g(u^{(i)})$
- want to predict unseen data between the 50 points



Solution approach

- linear model, square loss
- high-order polynomial feature embeddings with normalization
- standardization target embedding
- K-folds validation with $K = 10$
- two stages of regularization with hyperparameter tuning:
  - ◇ lasso to select important features
  - ◇ ridge to reduce model sensitivity to selected features

Embeddings

- start with 25th degree polynomial feature embedding:

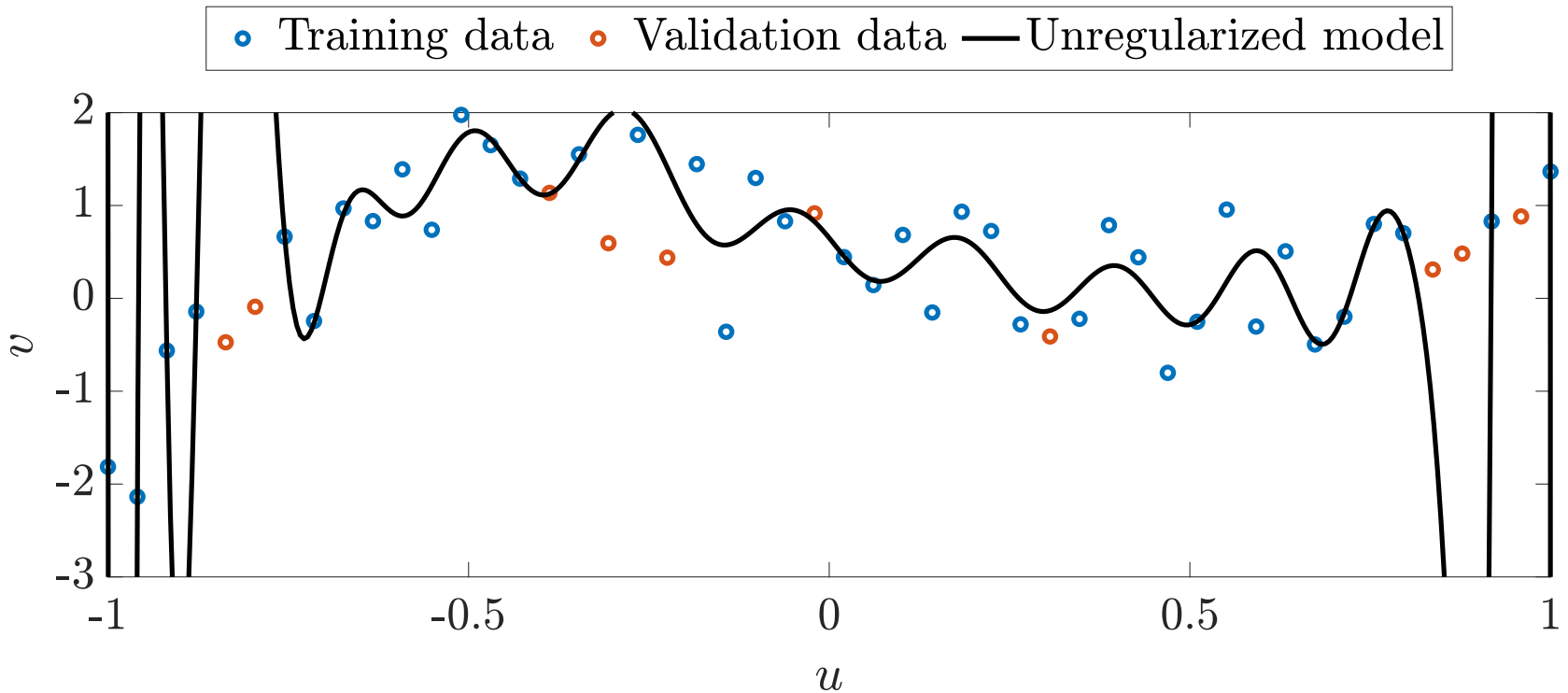
$$z^{(i)} = \begin{bmatrix} 1 \\ u^{(i)} \\ \vdots \\ (u^{(i)})^{25} \end{bmatrix}$$

- normalize the $z_2^{(i)}, \ldots, z_{26}^{(i)}$:

$$x^{(i)} = \begin{bmatrix} 1 \\ (z_2^{(i)} - \underline{z}_2)/(\overline{z}_2 - \underline{z}_2) \\ \vdots \\ (z_j^{(i)} - \underline{z}_{26})/(\overline{z}_{26} - \underline{z}_{26}) \end{bmatrix}$$

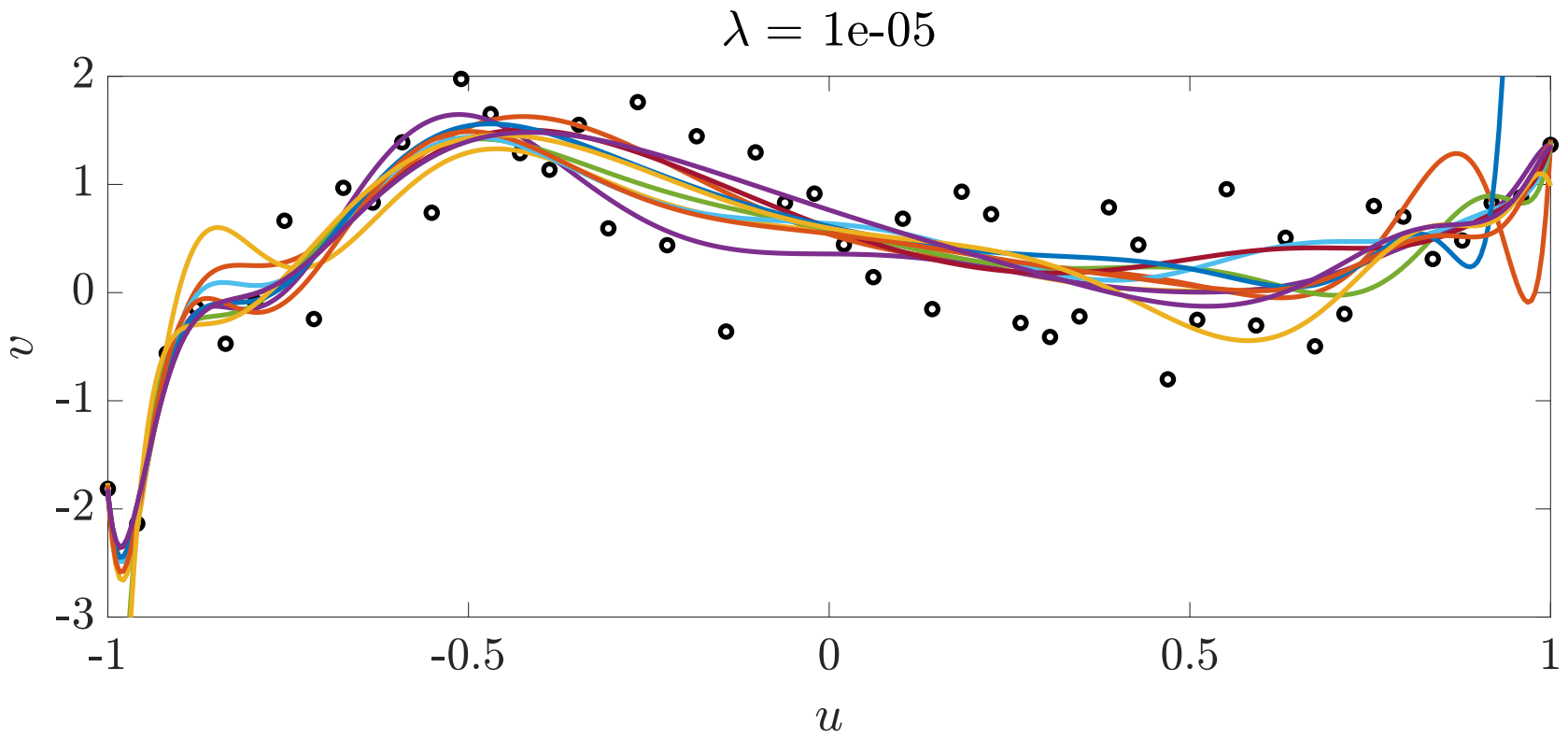
- standardize targets: $y^{(i)} = (v^{(i)} - \mu)/\sigma$

Unregularized model overfits training data



mean losses in fold 1: 0.188 training, 4,577 validation

Lasso-regularized models



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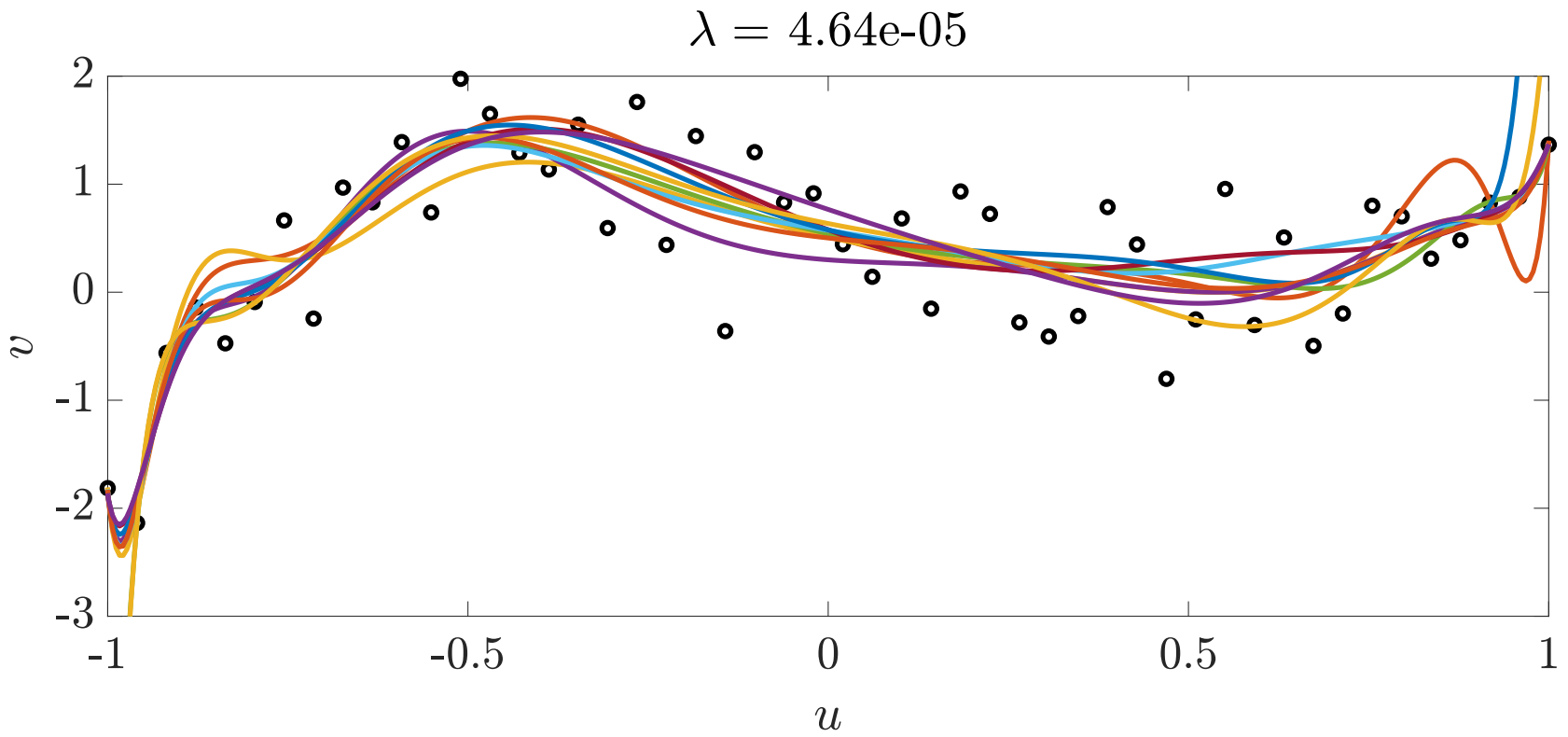

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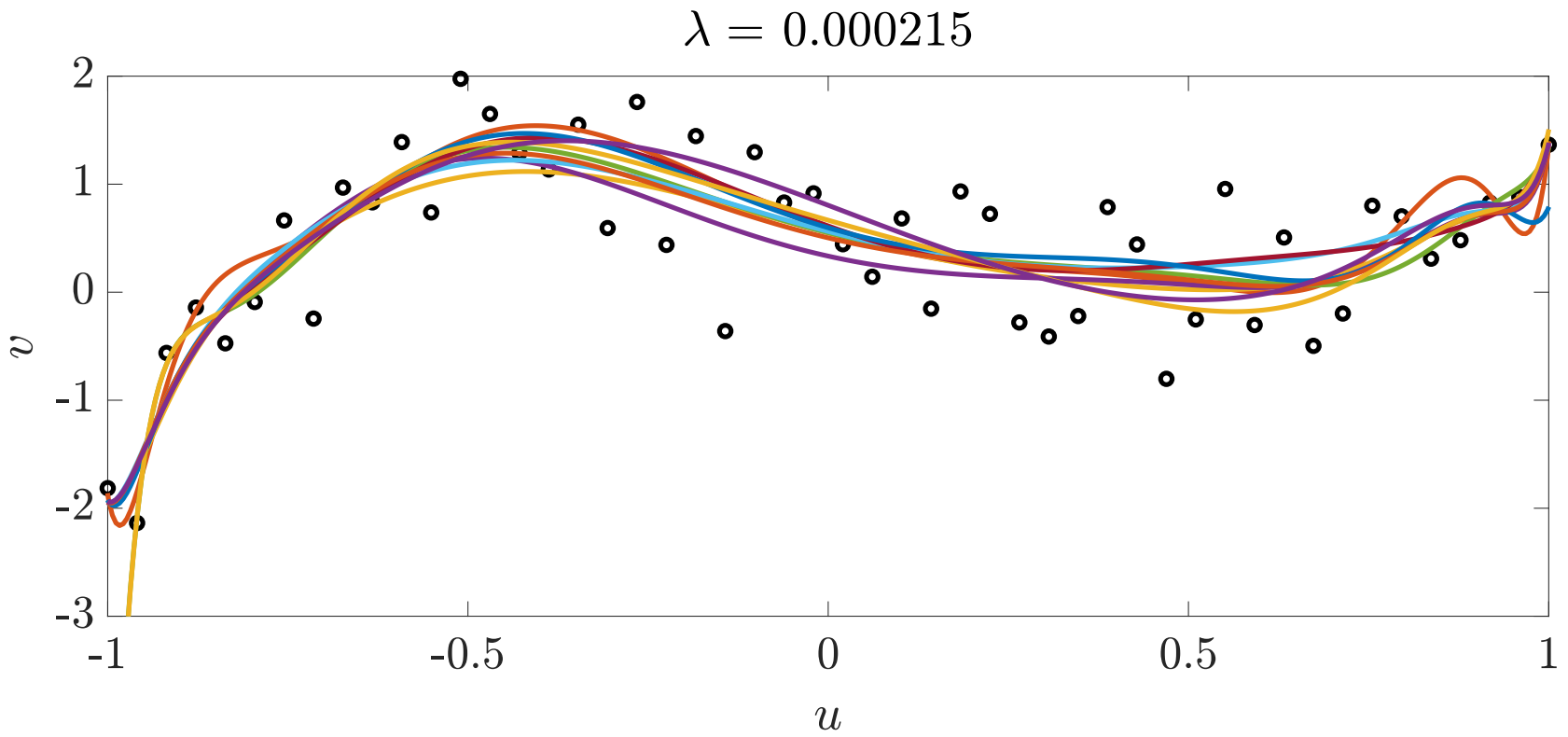

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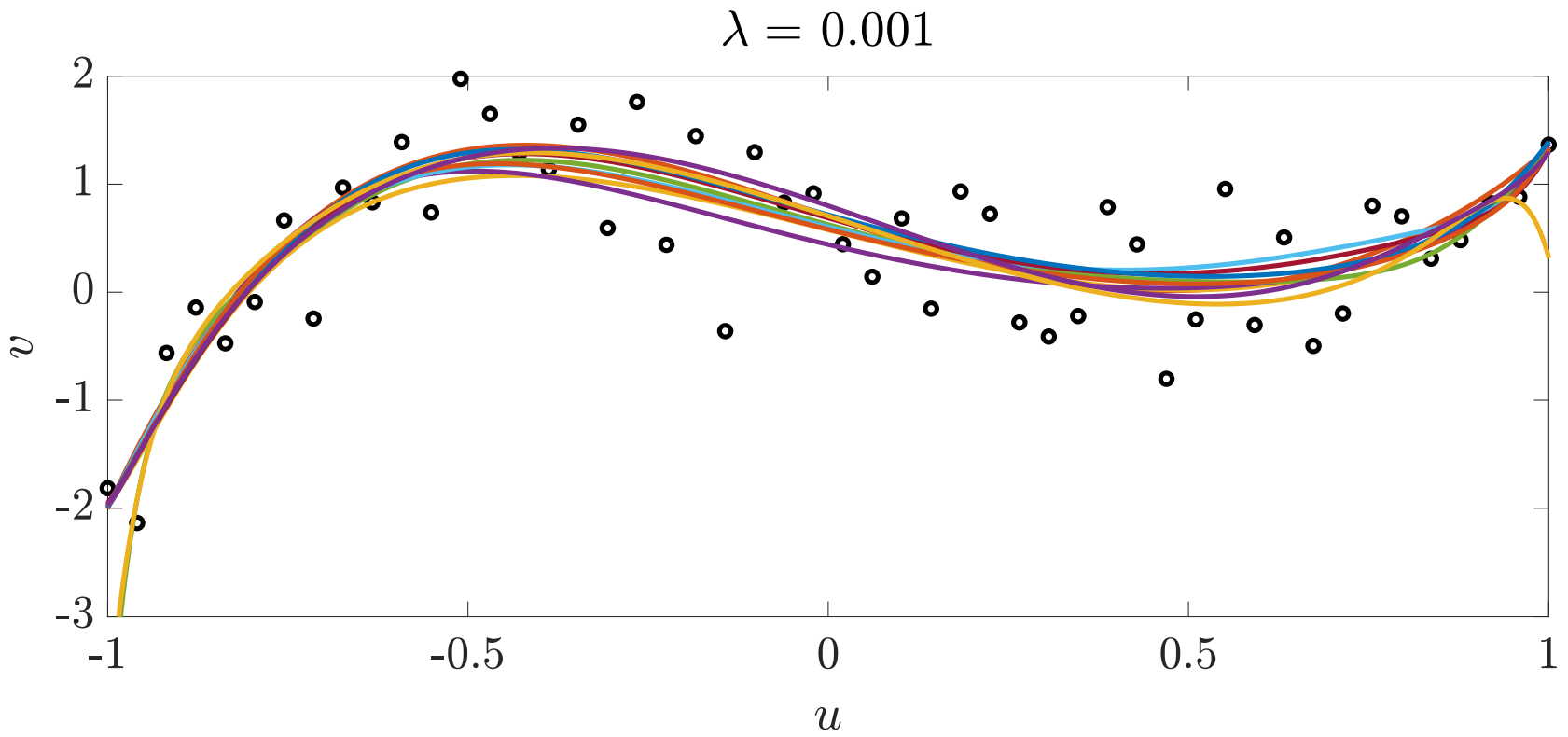

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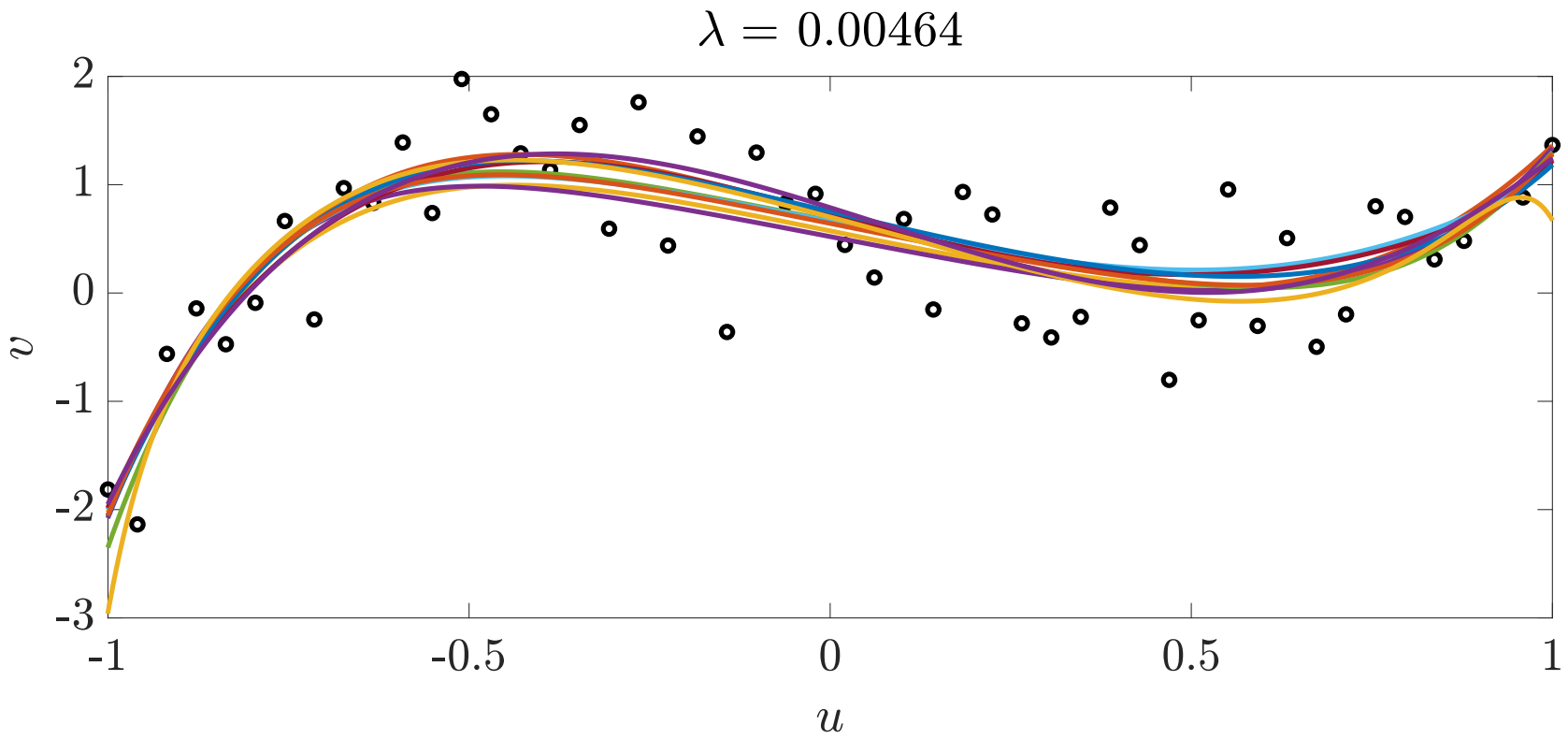

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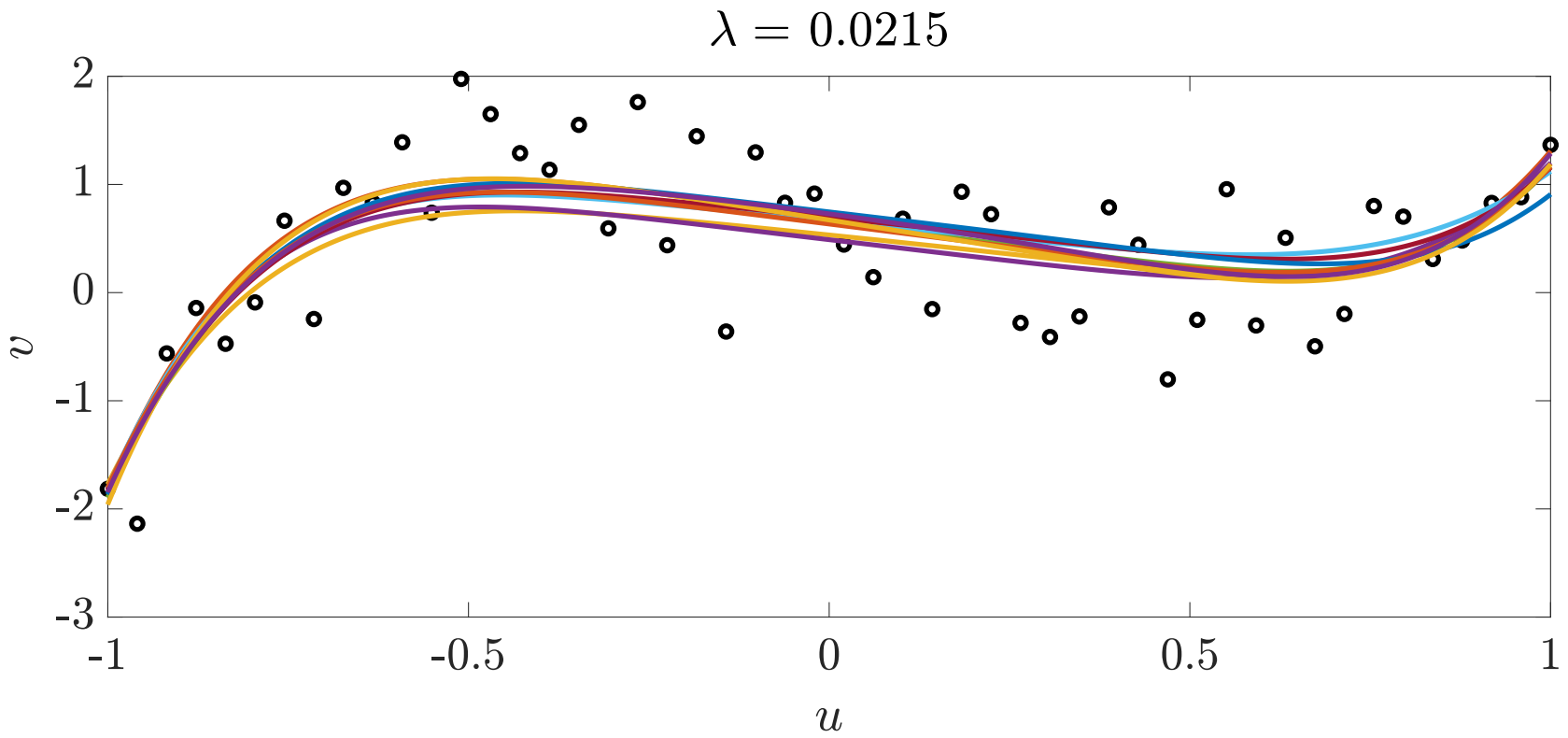

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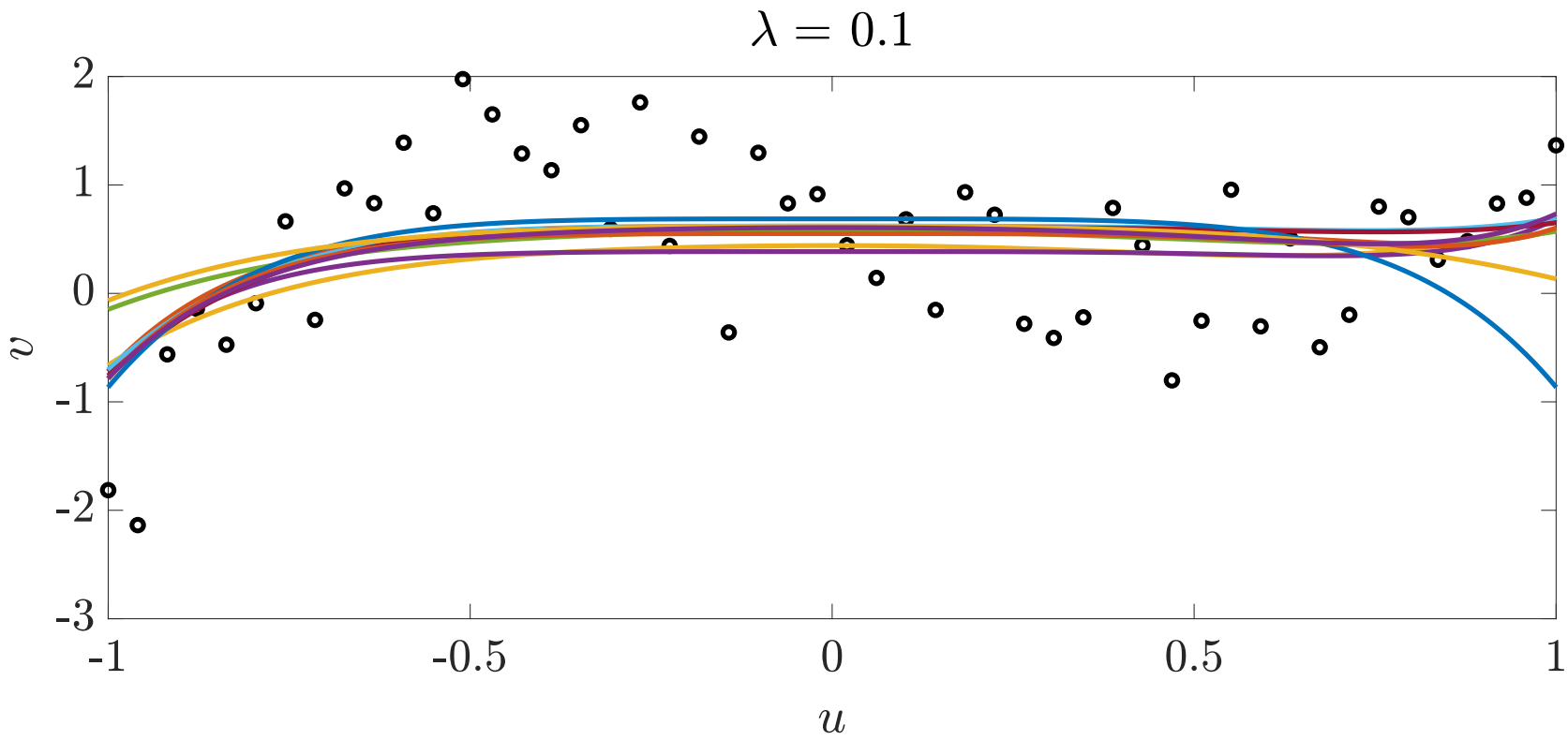

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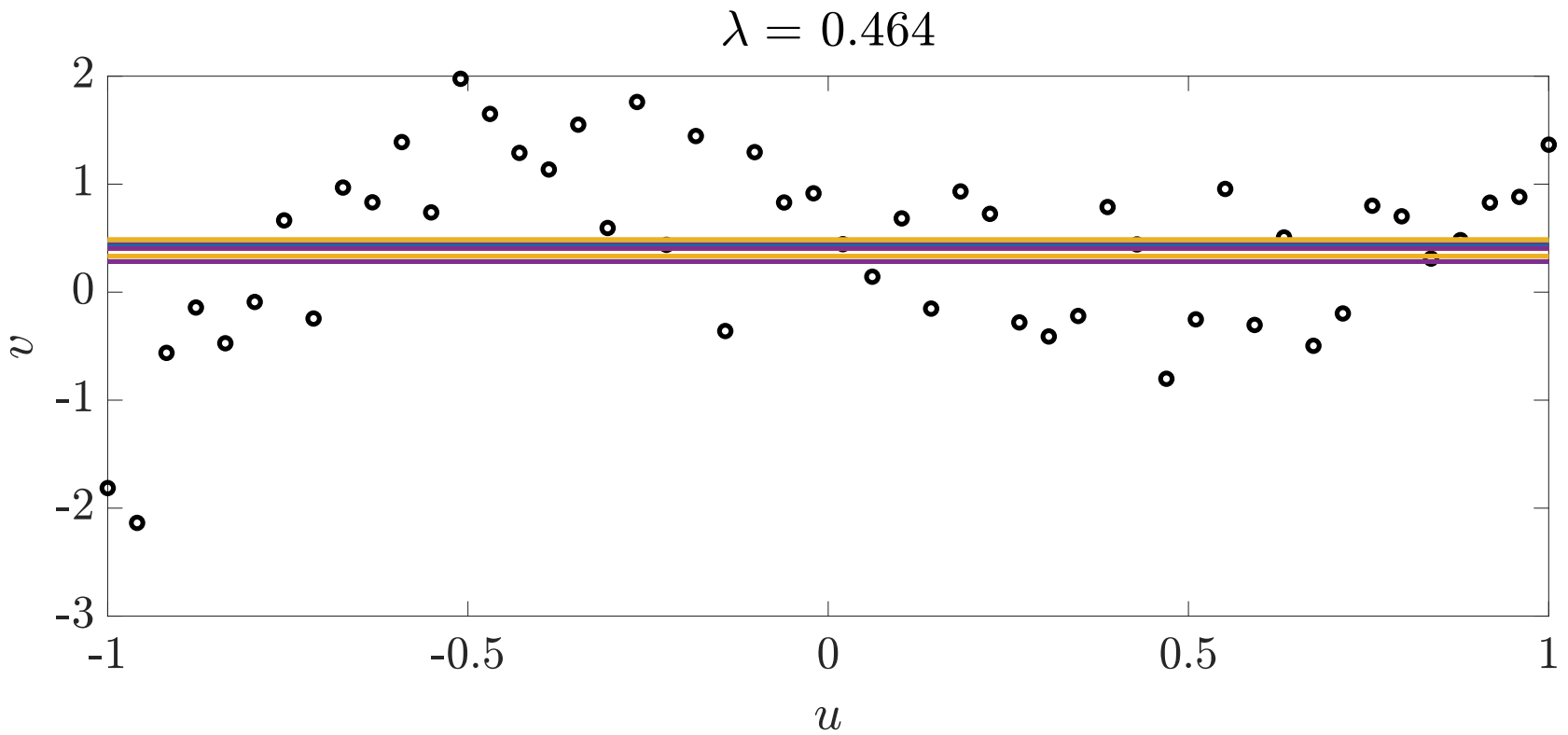

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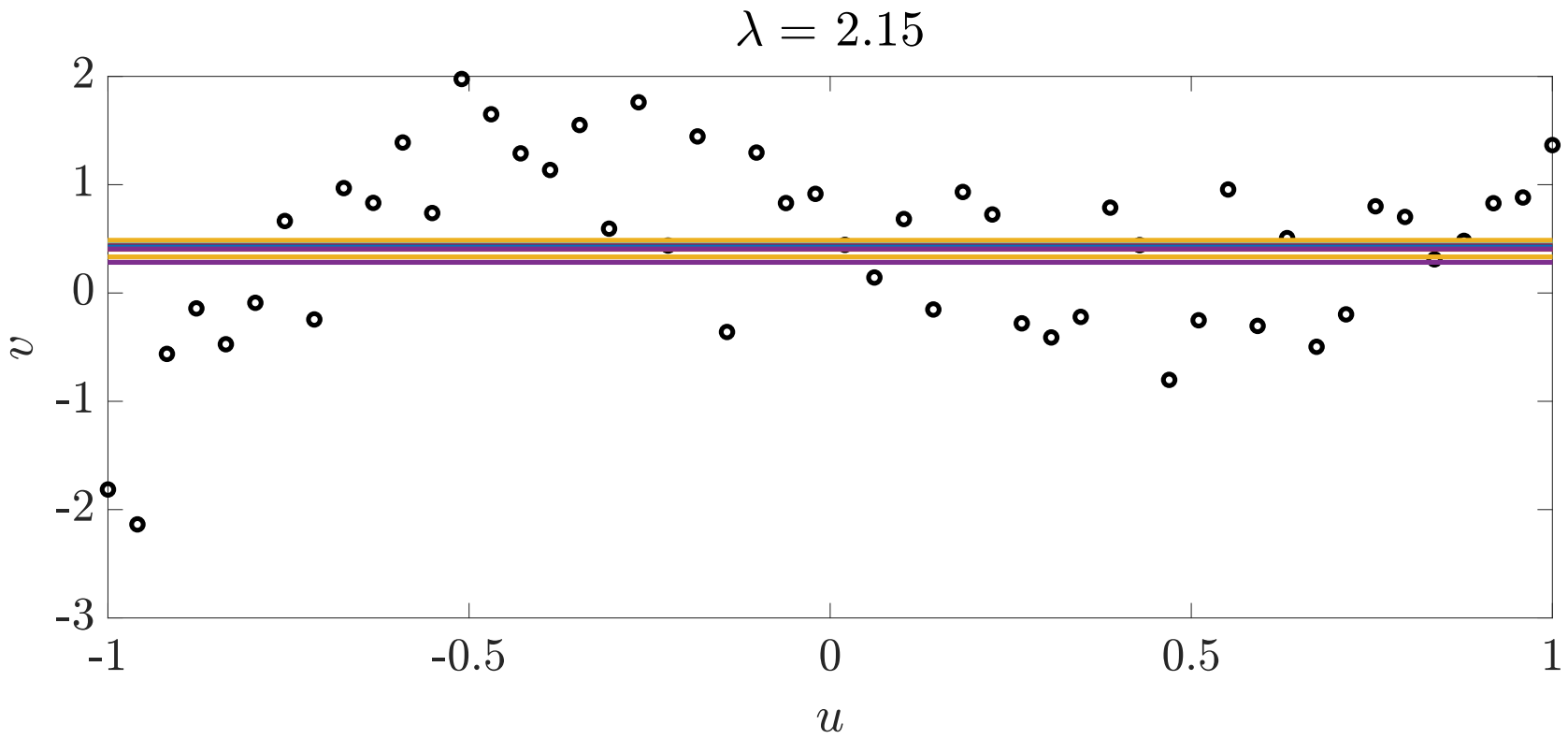

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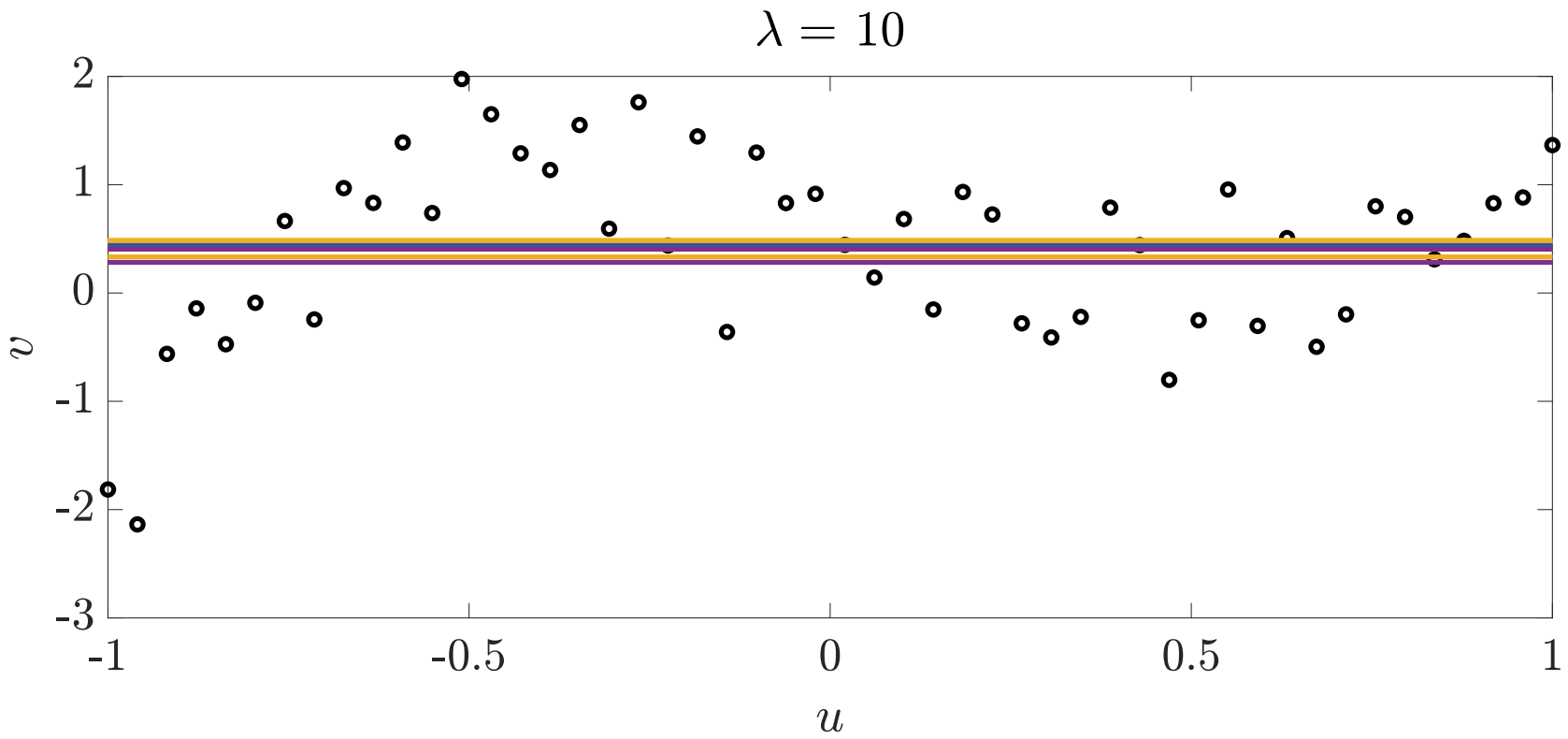
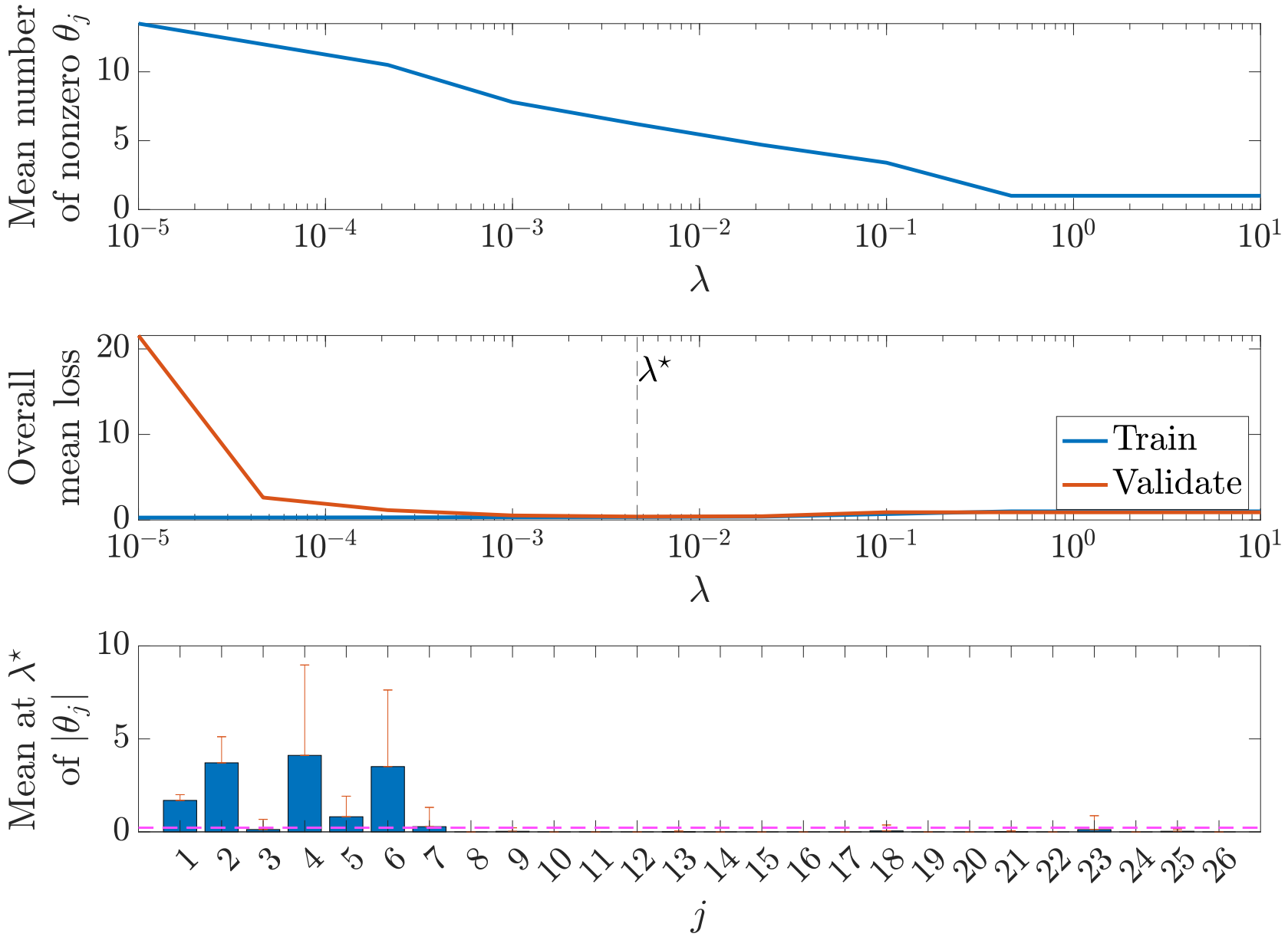
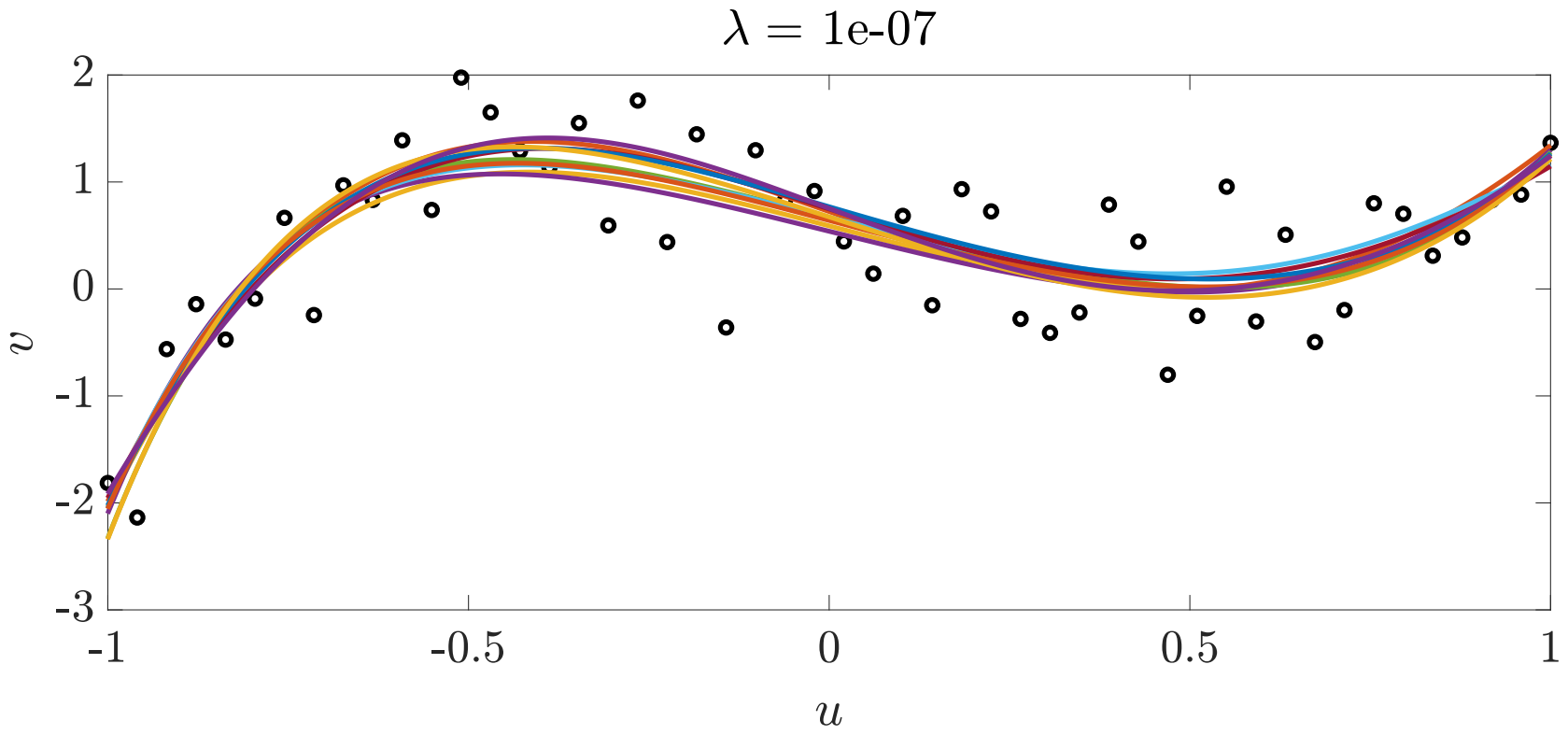


Feature selection via lasso regularization



Ridge-regularized models with selected features



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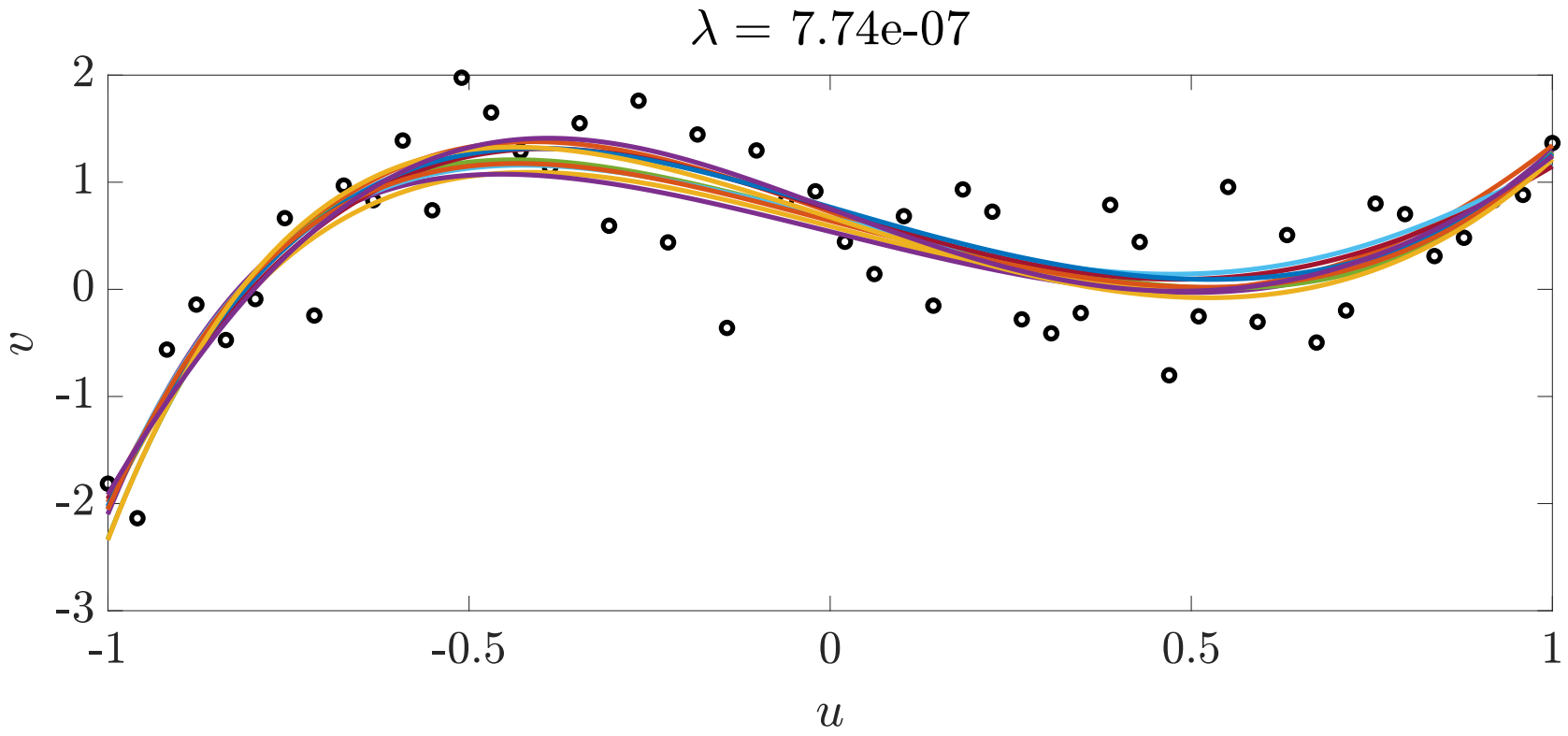

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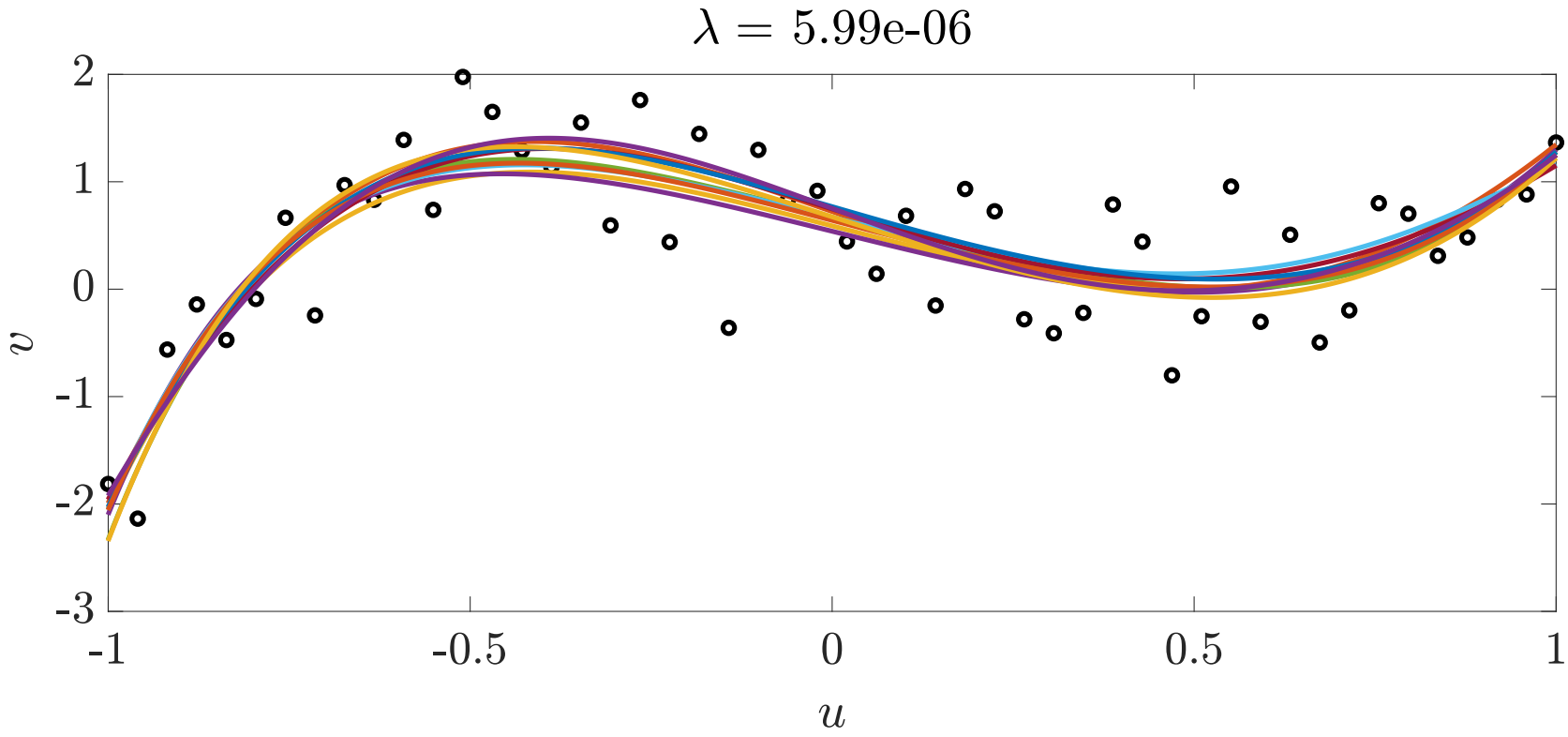

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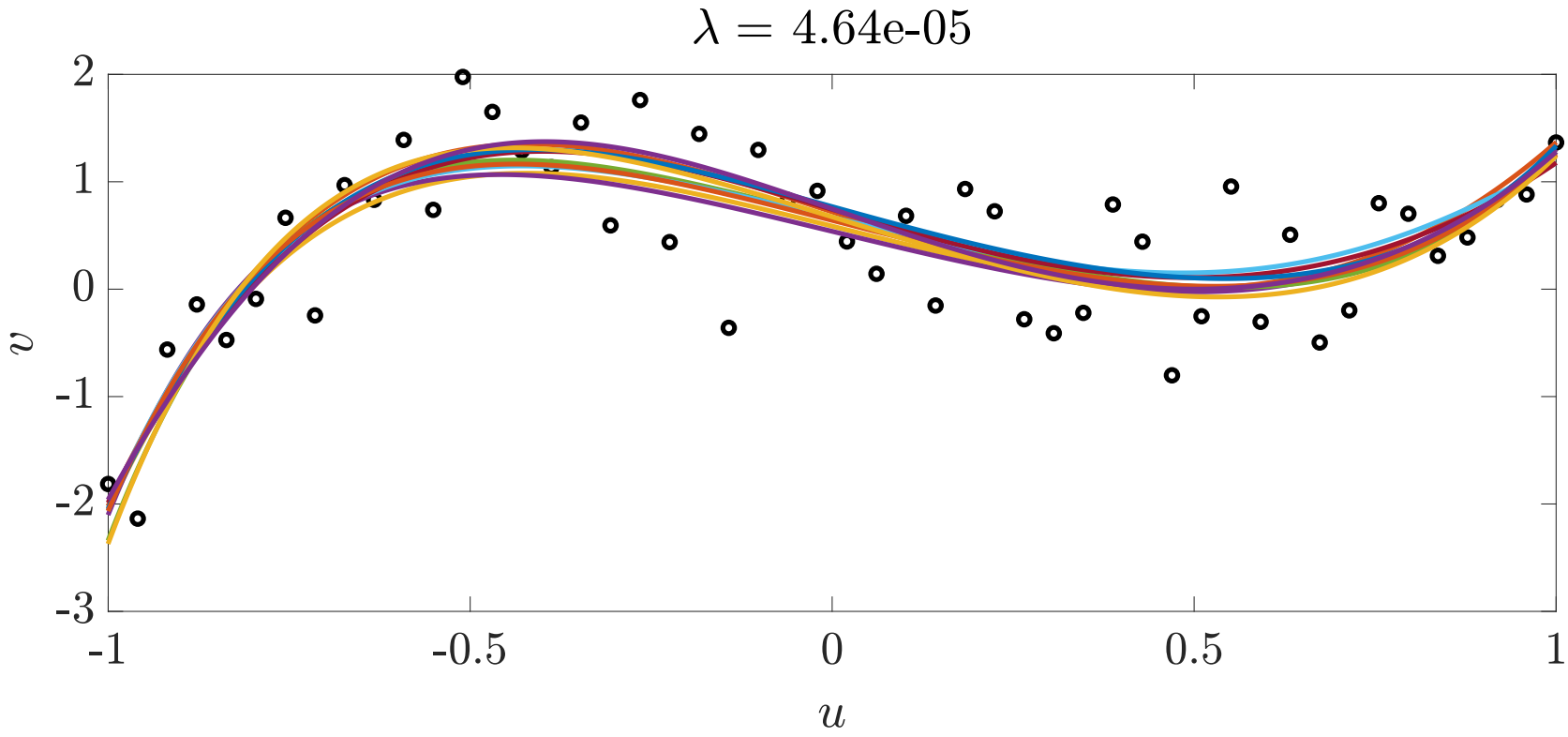

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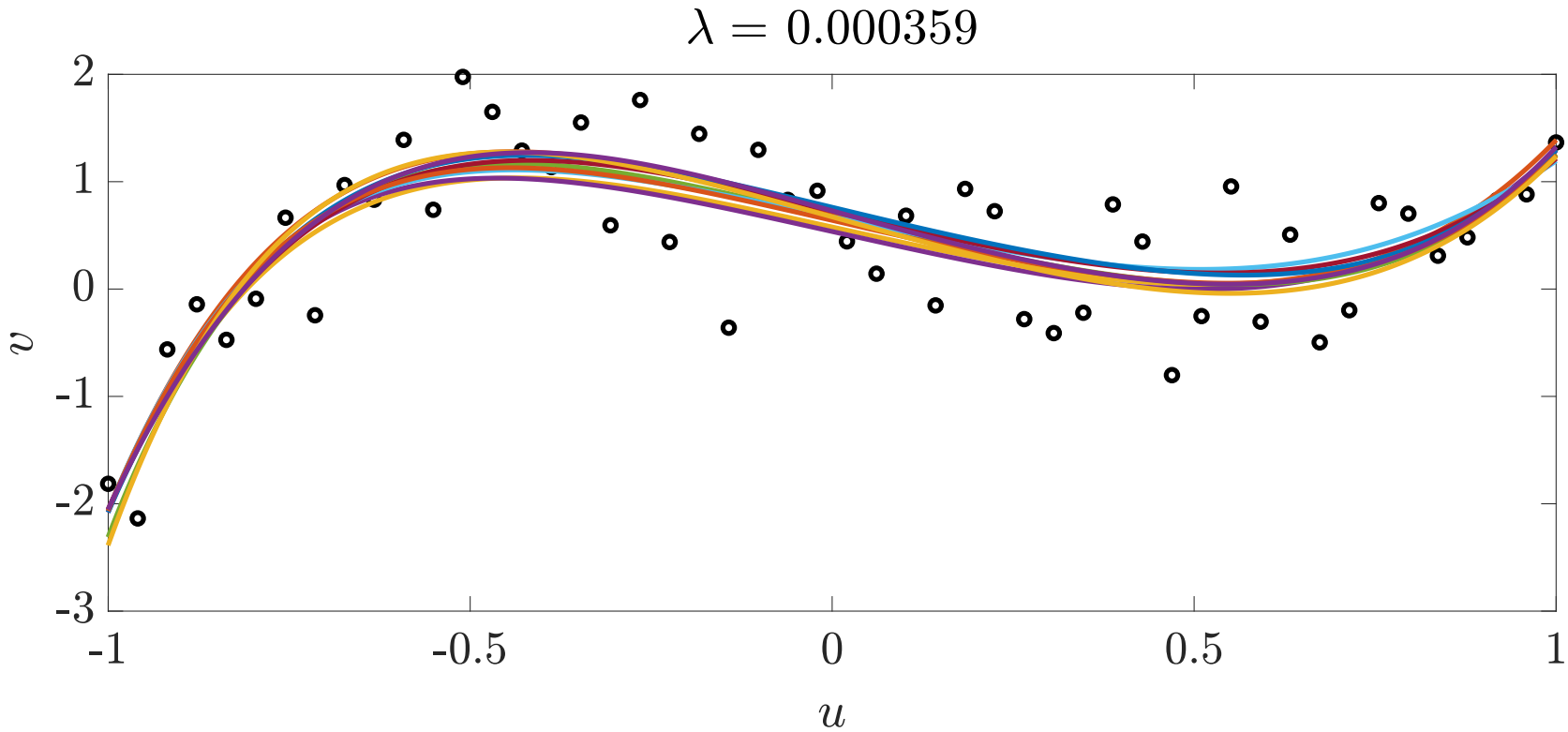

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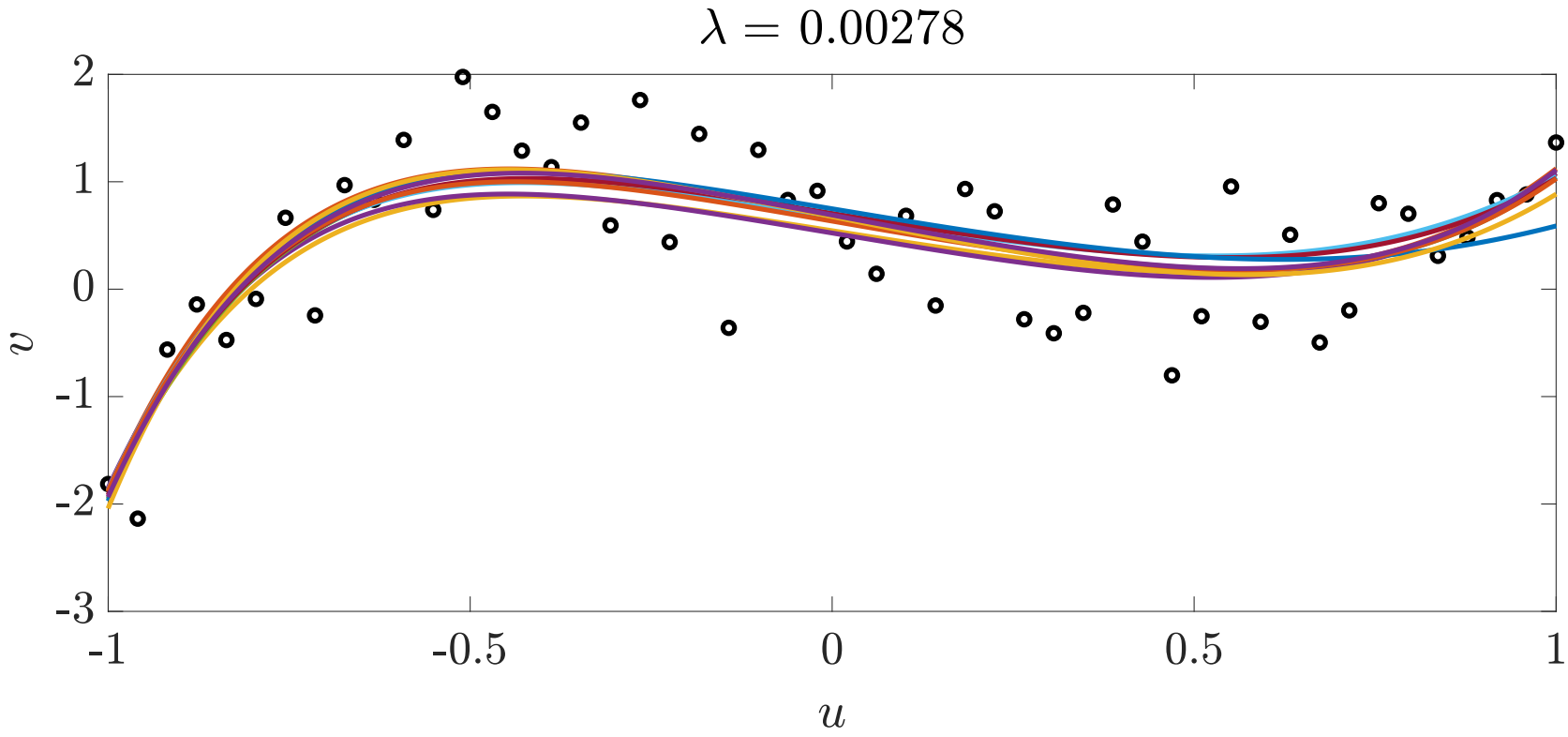

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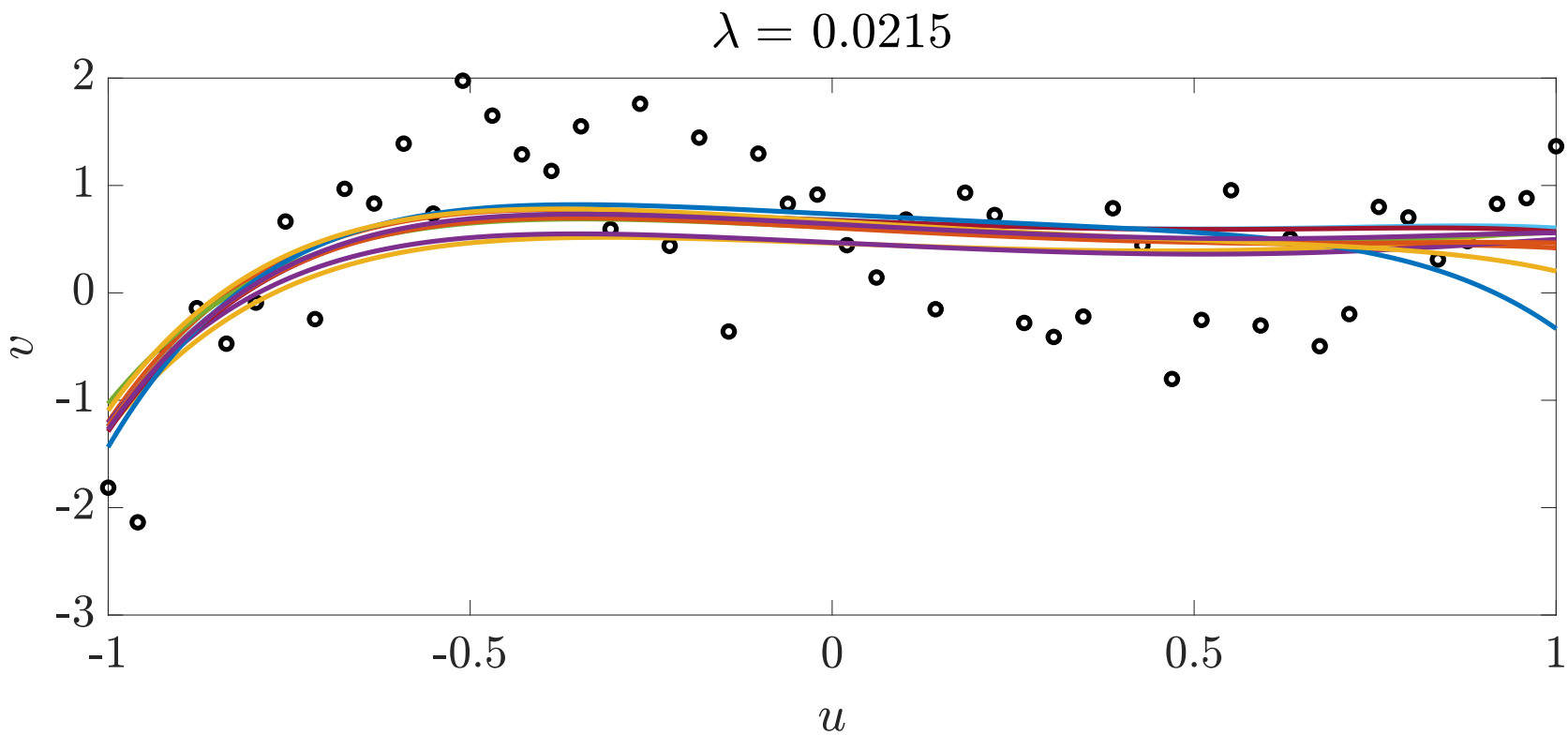

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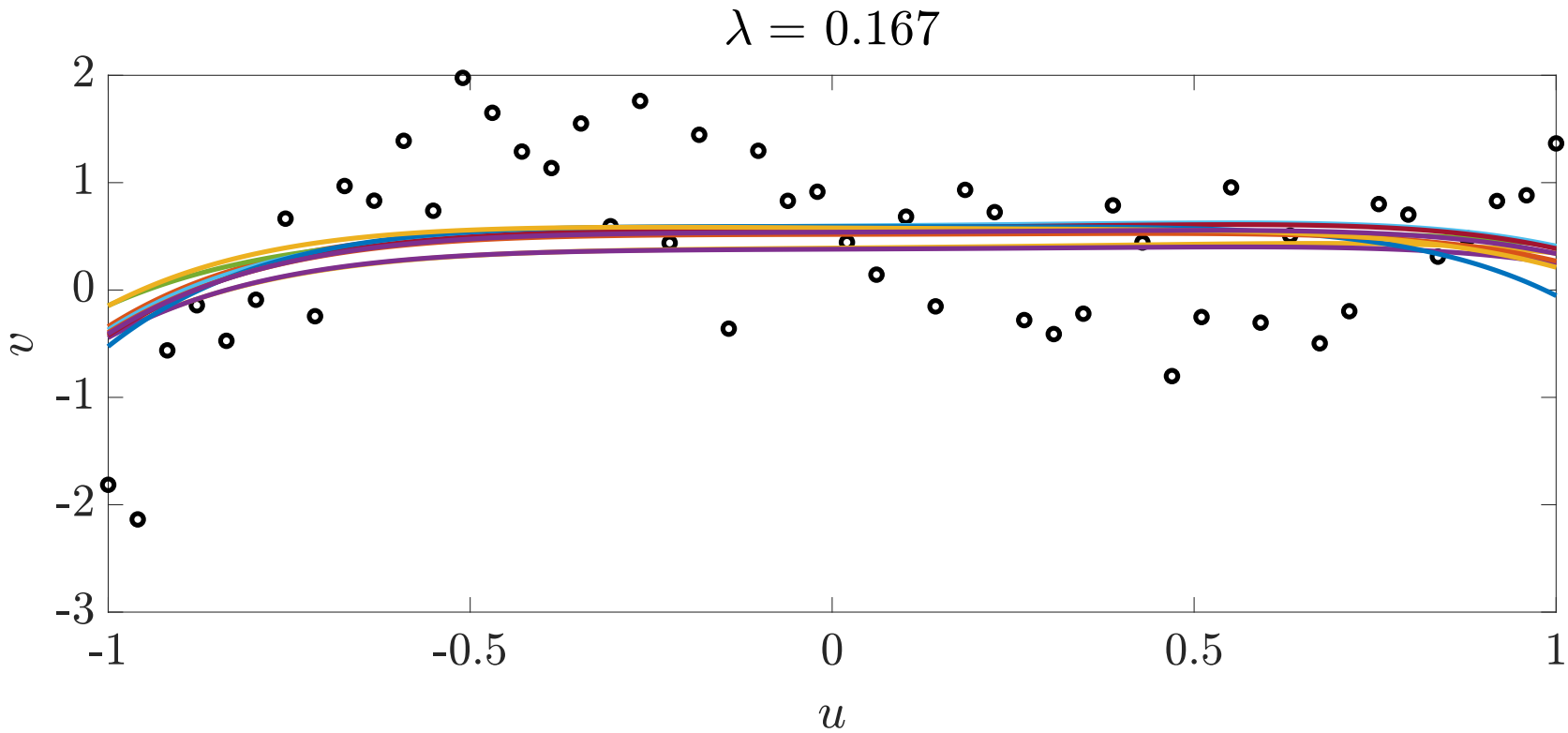

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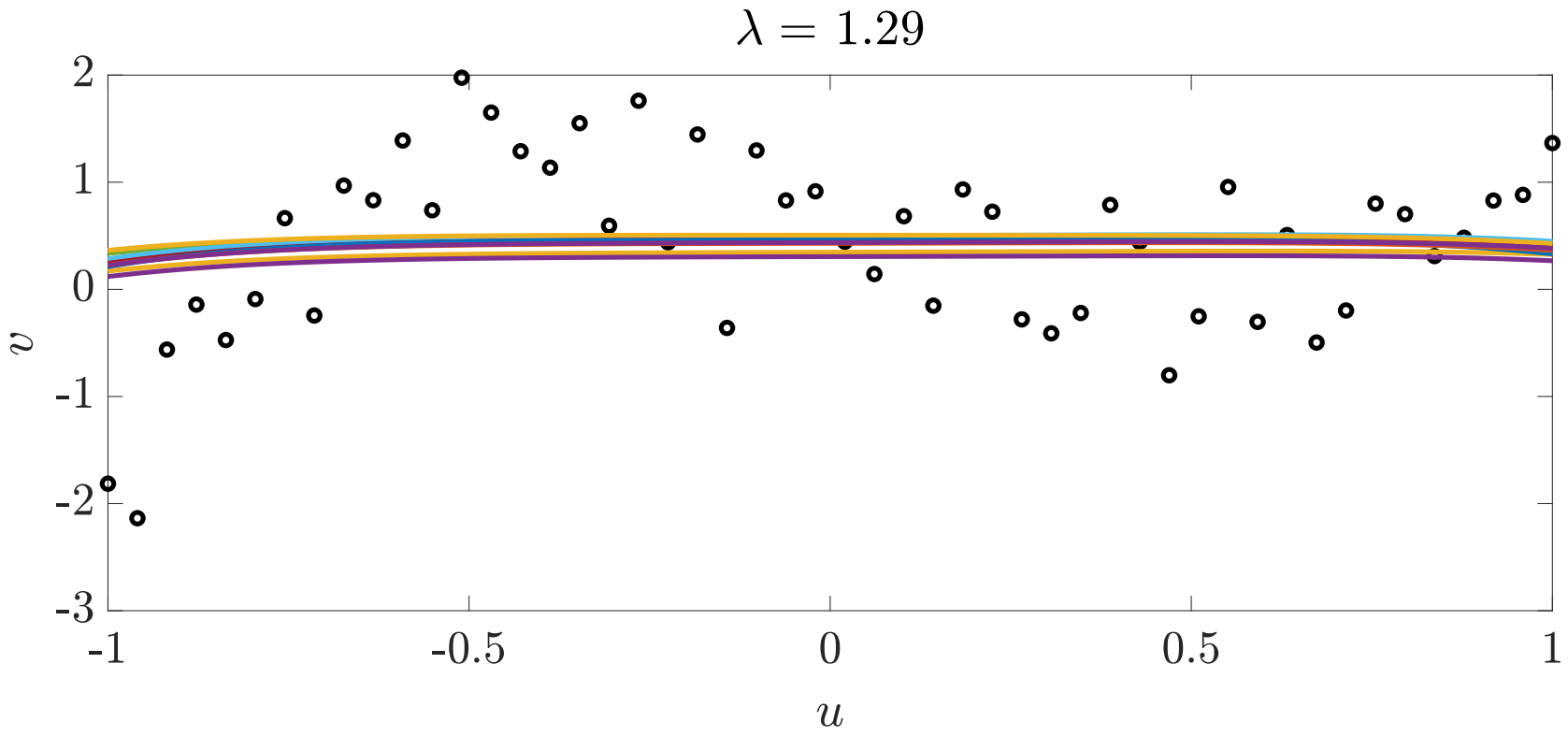

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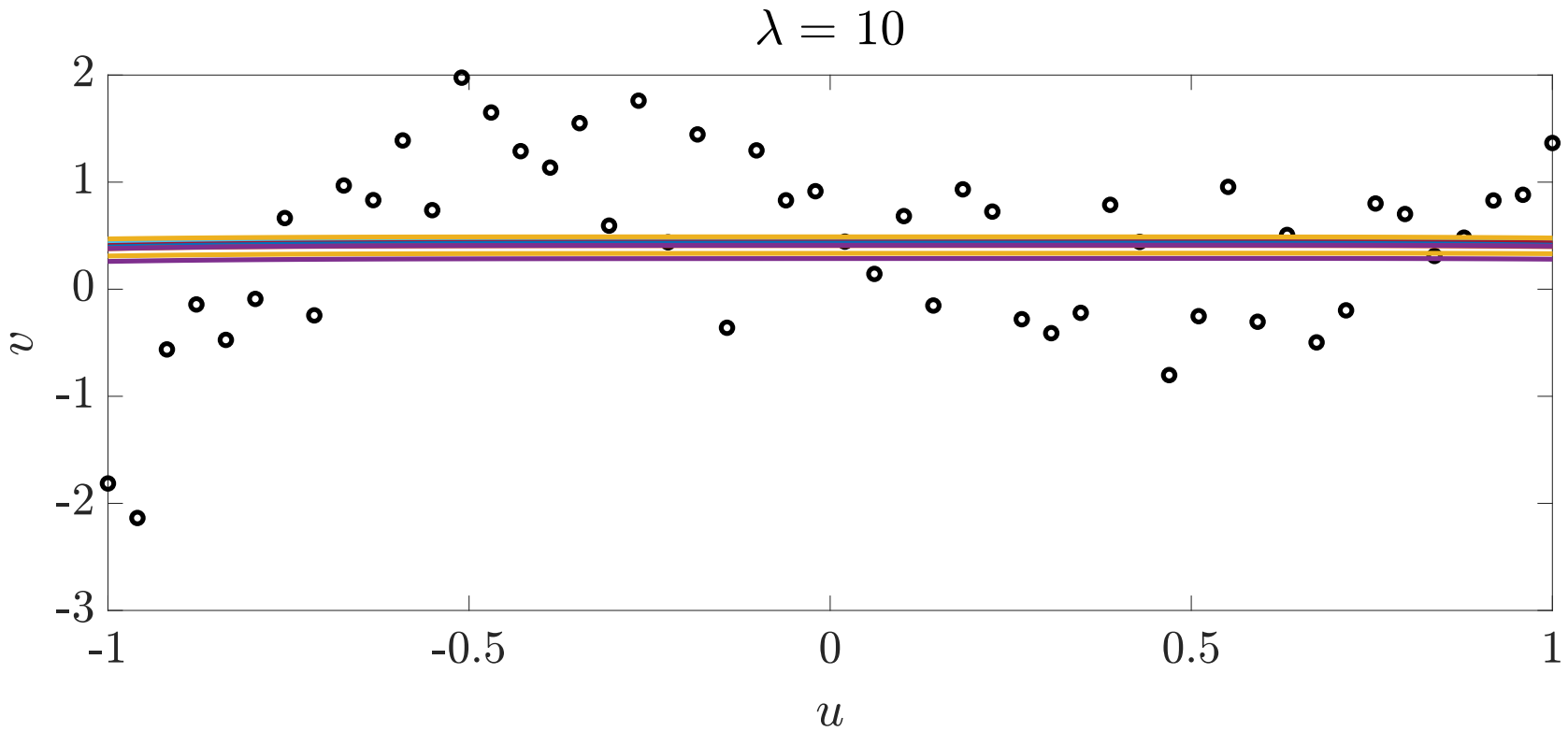
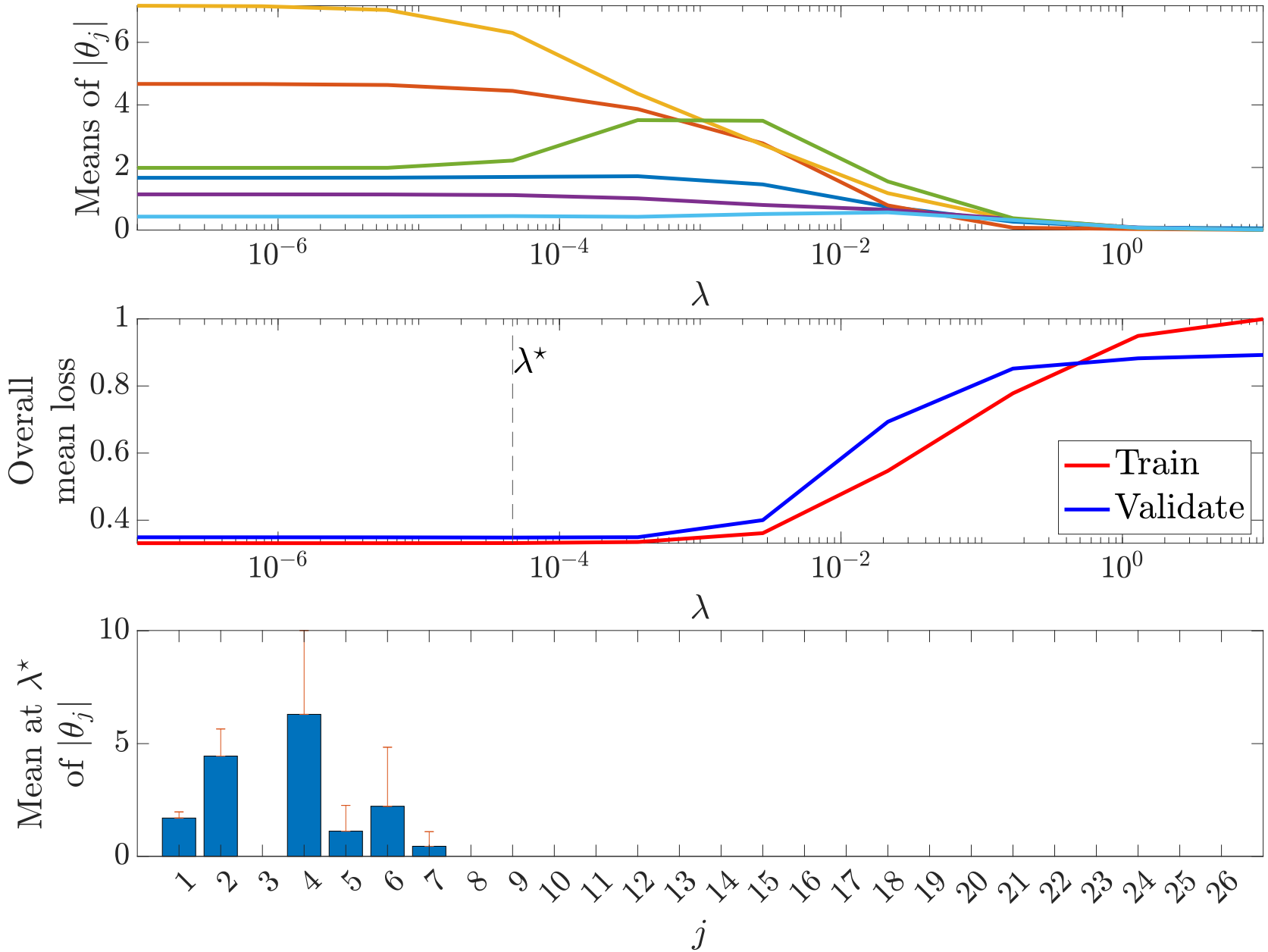
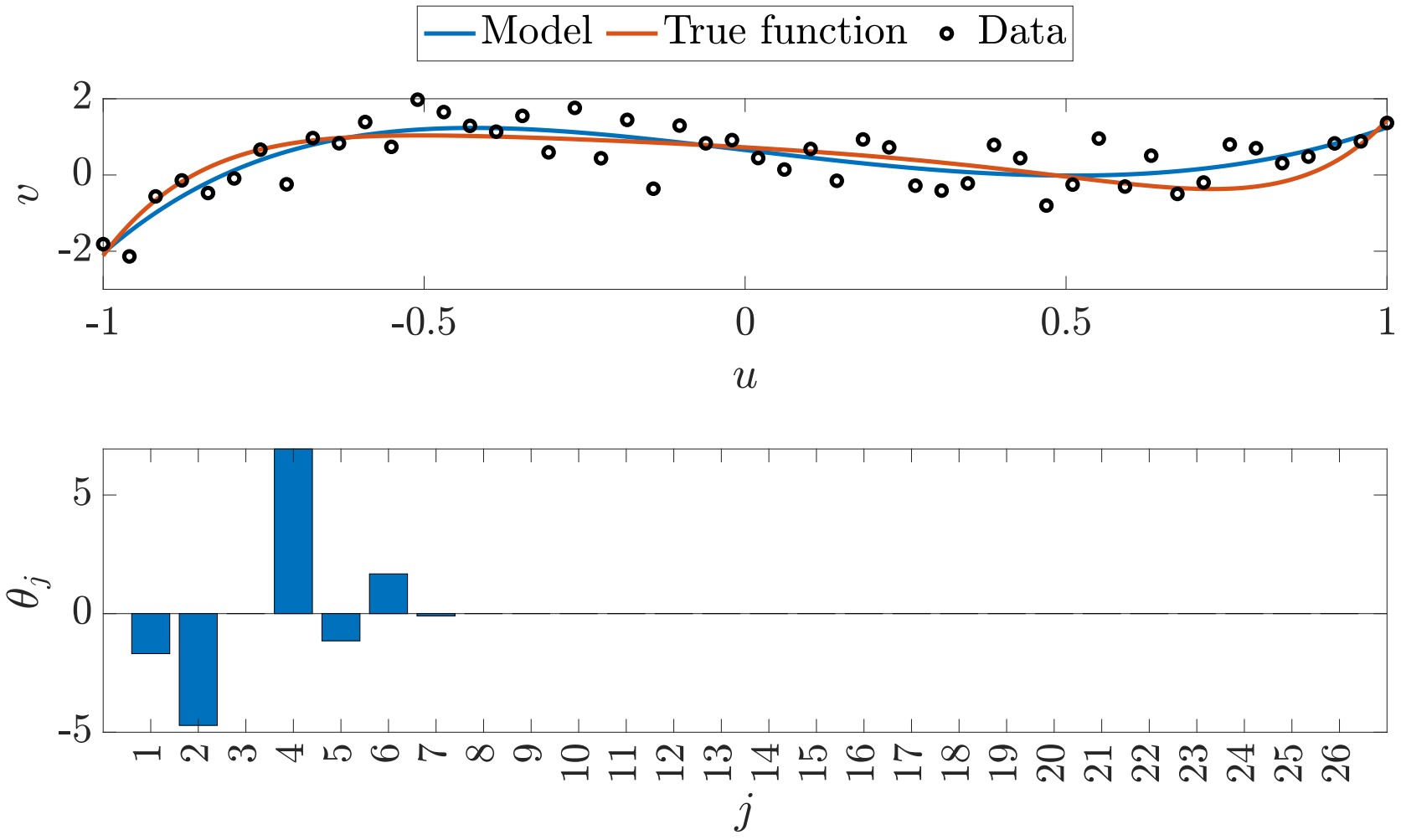


Hyperparameter tuning via ridge regularization



Final model


Model
True function
Data
2
0
-2
v
-1
-0.5
0
0.5
1
u
5
0
-5
θ_j
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
j

Summary

- 'linear models' are linear in θ and x, can be highly nonlinear in u
- general approach works for many problems
  1. embed raw inputs into a large number of candidate features
  2. select features via lasso regularization and K-folds validation
  3. 'polish' model with selected features and ridge regularization
- step 3 is fast (exact formula for square loss and ridge regularization)
- step 2 is slower (lasso regularization requires numerical optimization)
- approach also works for nonlinear models, but usually much slower

Outline

Problem

- estimate thermal resistance R in 1R1C building model,

$$C\frac{\mathrm{d}T(t)}{\mathrm{d}t} = \frac{T_{\text{out}}(t) - T(t)}{R} + q(t) + w(t)$$

- available measurements (5-minute time step, 6-week duration):
  - ◇ indoor temperature $T(t)$
  - ◇ outdoor temperature $T_{\text{out}}(t)$
  - ◇ heater thermal power $q(t)$

Prior information

- time-average of 1R1C model with $T(0) \approx T(\tau)$:

$$\frac{C}{\tau}\int_0^\tau \frac{\mathrm{d}T(t)}{\mathrm{d}t}\mathrm{d}t = \frac{1}{\tau}\int_0^\tau \left[\frac{T_{\text{out}}(t) - T(t)}{R} + q(t) + w(t)\right]\mathrm{d}t$$

$$\frac{C(T(\tau) - T(0))}{\tau} = \frac{\bar{T}_{\text{out}} - \bar{T}}{R} + \bar{q} + \bar{w}$$

$$\implies \bar{q} \approx \frac{\bar{T} - \bar{T}_{\text{out}}}{R} - \bar{w}$$

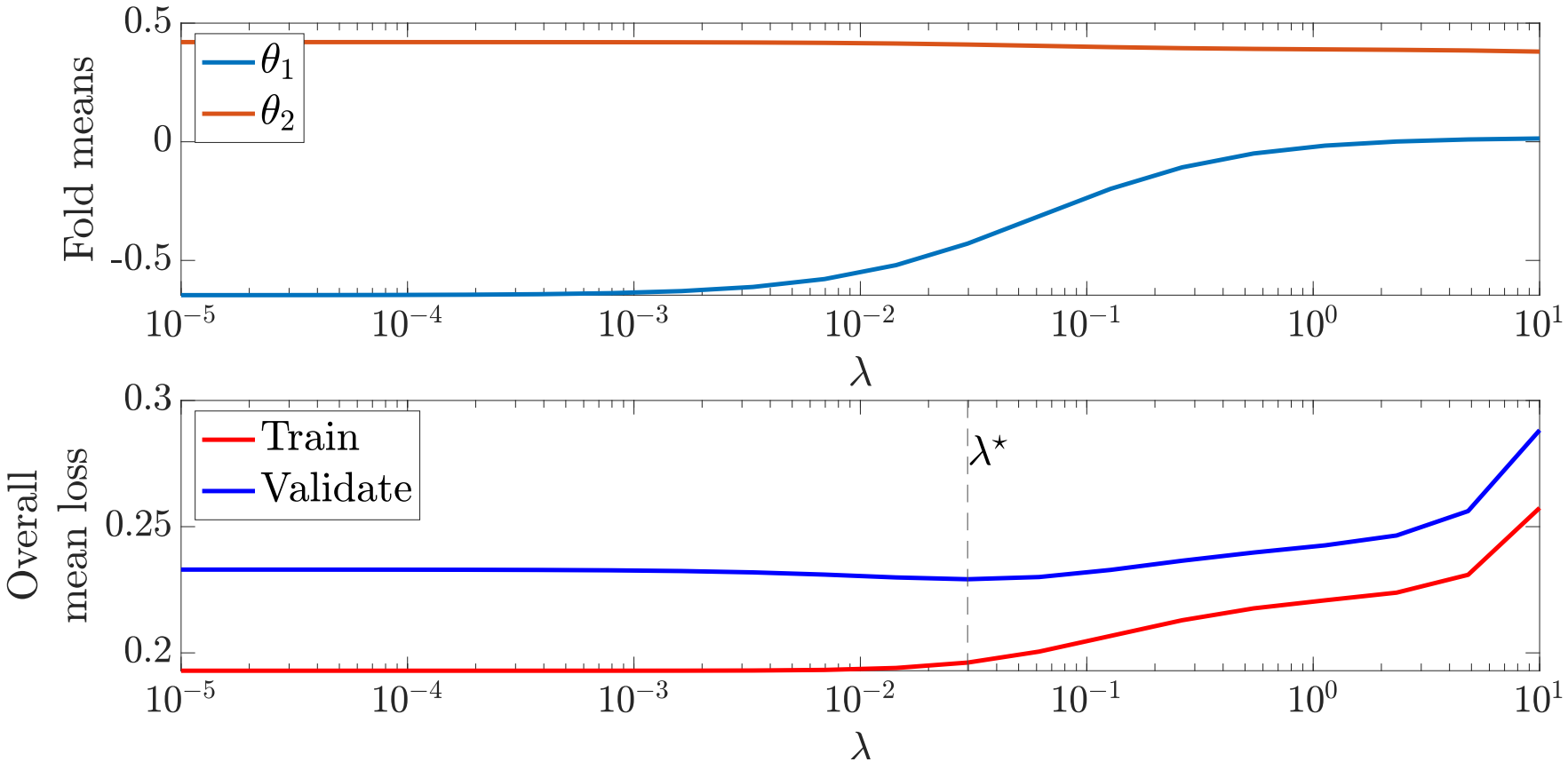
  where $\bar{q} = \frac{1}{\tau}\int_0^\tau q(t)\mathrm{d}t$ and so on for $\bar{T}$, $\bar{T}_{\text{out}}$, $\bar{w}$

- suggests linear model $y \approx \theta_1 x_1 + \theta_2 x_2$ with
  - ◇ target $y = \bar{q}$
  - ◇ features $x_1 = 1$, $x_2 = \bar{T} - \bar{T}_{\text{out}}$
  - ◇ parameters $\theta_1 = -\bar{w}$, $\theta_2 = 1/R$
- to avoid solar effects, embed raw data into nightly averages

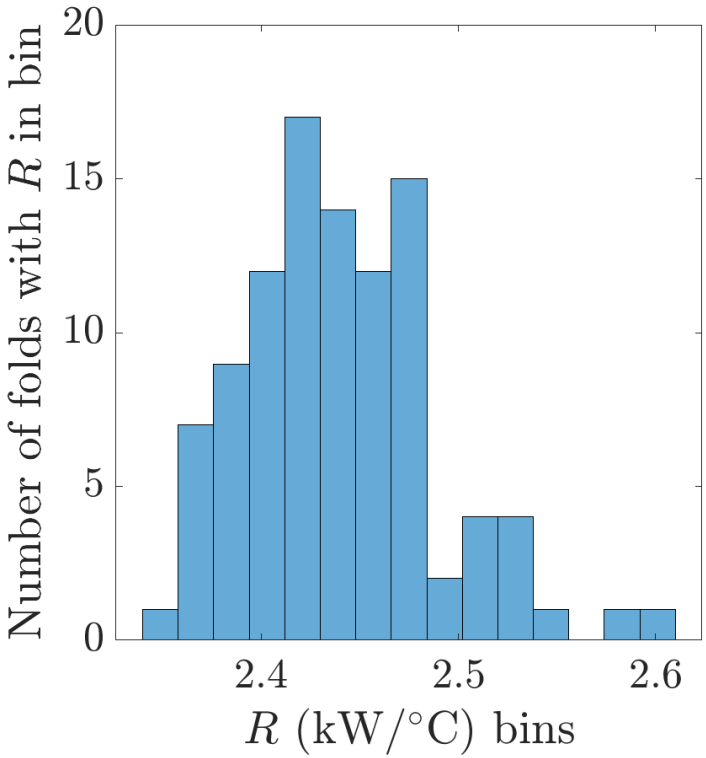
Solution approach

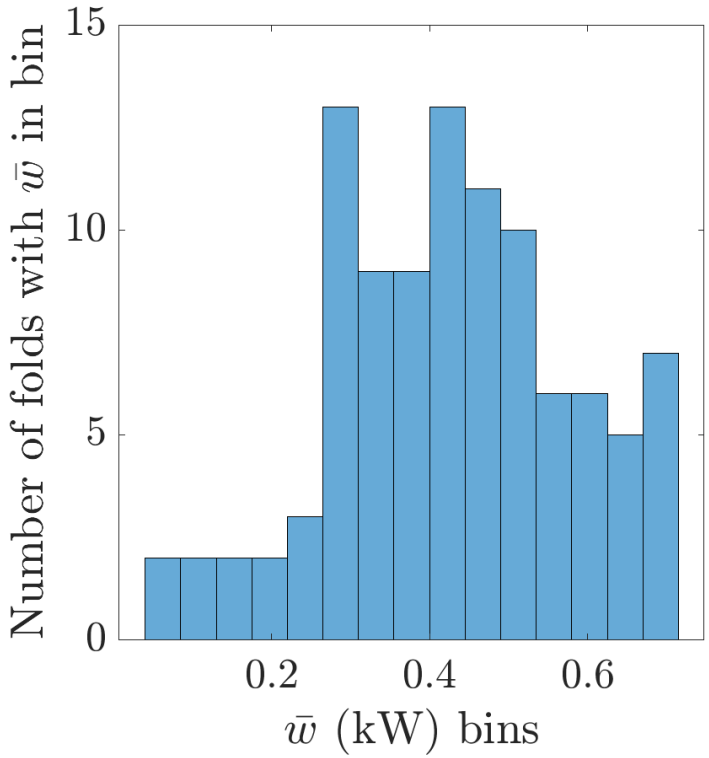
- linear model, square loss
- ridge regularization (including on constant feature)
- K-folds validation with $K = 100$
- only 2 features, so no need for a feature selection step

Hyperparameter tuning



Histograms of parameter estimates at $\lambda^\star$





Final model, retrained on all (training + validation) data