Model selection and validation

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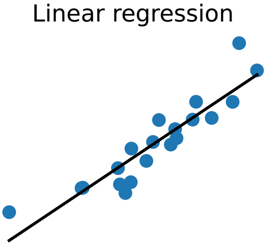
MAIN educational 2022-12-10

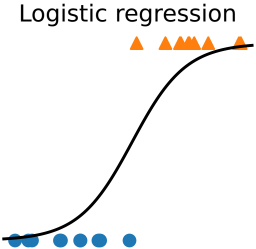
Outline

Recap of part 1

Supervised learning

- Regression: least-squares linear regression
- Classification: logistic regression





Recap of part 1

Supervised learning

- Regression: least-squares linear regression
- Classification: logistic regression

Regularization

- ℓ_2 a.k.a. ridge regularization

Recap of part 1

Supervised learning

- Regression: least-squares linear regression
- Classification: logistic regression

Regularization

- ℓ_2 a.k.a. ridge regularization

Model evaluation and selection

- Out-of-sample generalization; independent test set
- Performance metrics:
  - regression: mean squared error
  - classification: accuracy, ROC curve
- Cross-validation

Notation & vocabulary

Supervised learning framework

$$Y = f(X) + E \tag{1}$$

- $Y \in \mathbb{R}$: output (a.k.a. target, dependent variable) to predict

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- $E \in \mathbb{R}$: unmodelled noise

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- $E \in \mathbb{R}$: unmodelled noise
- f: the function we try to approximate

Example (Linear regression)

$$\begin{align} Y &= \beta_0 + \langle X, \beta \rangle + E \tag{2} \\ &= \beta_0 + \sum_{j=1}^{p} X_j \, \beta_j + E \tag{3} \end{align}$$

"learning" = choosing $\beta_0 \in \mathbb{R}$ and $\boldsymbol{\beta} \in \mathbb{R}^p$

How to set parameters: Empirical Risk Minimization

- Choose a loss function L measuring how bad is our error.
- Example: squared error $L(Y, \hat{Y}) = (Y - \hat{Y})^2$, where $\hat{Y}$ is the prediction
- We want to minimize the expected error (risk): $\mathbb{E}[L(Y, \hat{Y})]$

How to set parameters: Empirical Risk Minimization

We do not know the risk: estimate it from a sample.
Given n training examples $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$, minimize the empirical risk: $\sum_{i=1}^{n} L(y_i, \hat{y}_i)$

For linear regression:
find $\hat{\beta}_0 \in \mathbb{R}, \hat{\boldsymbol{\beta}} \in \mathbb{R}^p$ that minimize

$$\|y - \hat{y}\|_2^2 = \|y - \hat{\beta}_0 - X\,\hat{\boldsymbol{\beta}}\|_2^2 \tag{4}$$

$$= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j=1}^{p} X_{ij}\,\hat{\boldsymbol{\beta}}_j)^2 \tag{5}$$

"Fitting" the parameters to X, y.

Evaluating a model

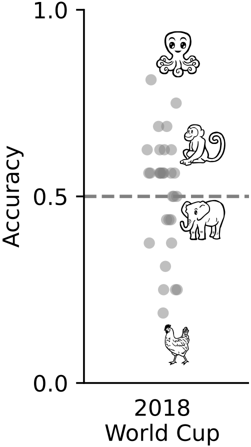
We always want to do 2 distinct things:

- Select a model (set the parameters).
- Evaluate its performance.

We can never do both on the same data!

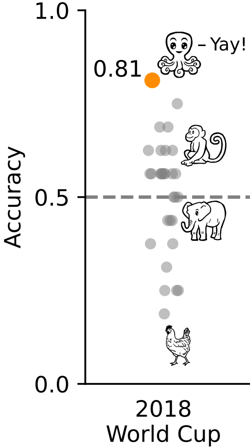
Training error is a biased estimator of the risk

- 30 different animals made predictions about match results in the 2018 World Cup



Training error is a biased estimator of the risk

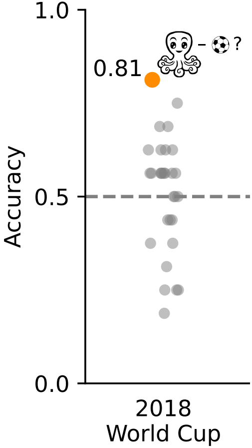
- 30 different animals made predictions about match results in the 2018 world cup
- We **selected the best predictor** (highest accuracy)



Training error is a biased estimator of the risk

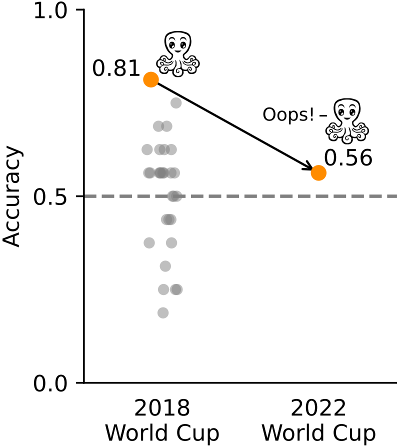
The same animal is invited to make predictions about the 2022 World Cup. Is it more likely to perform:

1. Better than in 2018?
2. Worse than in 2018?
3. The same?



Training error is a biased estimator of the risk

The selected animal is more likely to perform **worse** than in 2018.



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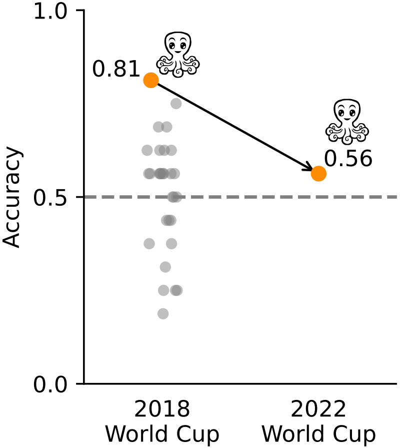
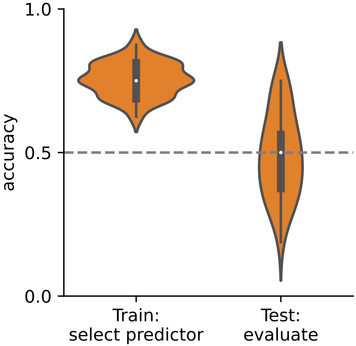


Its 2018 performance is a **biased** estimator of its expected performance in future World Cups.

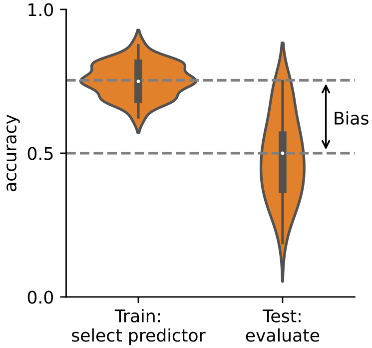
Training error is a biased estimator of the risk

Distribution of train and test errors across 50 repetitions:



Training error is a biased estimator of the risk

- The systematic difference is the bias.
- It is why we cannot use the training error to estimate model performance.



Estimating prediction performance

When you hear "best", "maximum", "select", ... think "bias"

Setting the parameters

- **Select** β that gives the **best** prediction on training data
- The prediction score for $\hat{\beta}$ is biased: compute a new score on unseen test data.

scikit-learn "estimator API": `fit`; `predict`

```
estimator = Ridge()
estimator.fit(X_train, y_train)
predictions = estimator.predict(X_test)
```

Scikit-learn user guide
`sklearn.linear_model.Ridge`

("API": "Application Programming Interface" – the specific way in which the library exposes its behaviour to user code: method names & signatures, etc.)

Evaluating performance with sklearn.metrics

```
estimator = Ridge()
estimator.fit(X_train, y_train)
predictions = estimator.predict(X_test)

mse = metrics.mean_squared_error(y_test, predictions)
```

sklearn.linear_model.Ridge
sklearn.metrics
User guide on model evaluation

ex_01_fit_predict_questions.py

Some possible metrics for regression

R^2 score (coefficient of determination): `r2_score`

$$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} , \tag{6}$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$

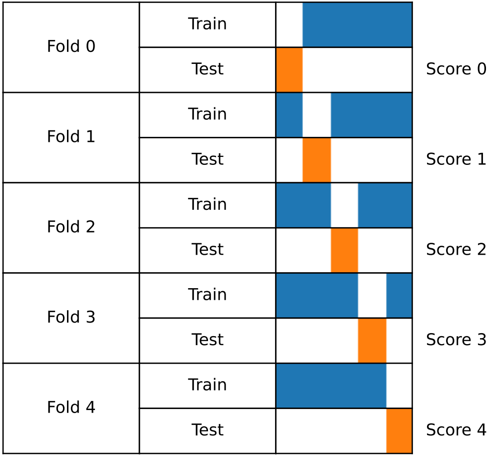
Mean Squared Error (MSE): `mean_squared_error`

$$\mathrm{MSE}(y, \hat{y}) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{7}$$

Mean Absolute Error (MAE): `mean_absolute_error`

$$\mathrm{MAE}(y, \hat{y}) = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{8}$$

Cross-validation



User guide on cross-validation

`sklearn.model_selection.cross_validate`

`sklearn.model_selection.cross_val_score`

`ex_02_cross_validate_questions.py`

Outline

Introduction: cross-validation

Model and hyperparameter selection

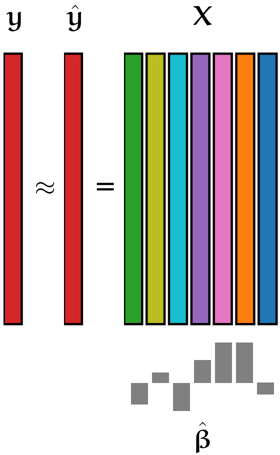
Dimensionality reduction

Conclusion: summary of pitfalls

Need for regularization

Linear regression: projection on the column space of X

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}} \qquad (9)$$



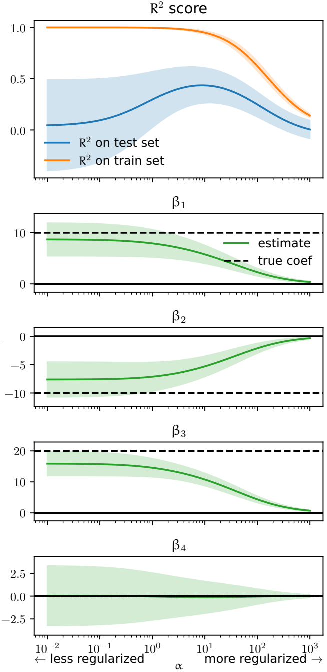
- Too many features: high variance & unstable solution
- Solutions: **regularization**, dimensionality reduction

Regularization

Example (Ridge regression)

$$\underset{\boldsymbol{\beta}, \beta_0}{\operatorname{argmin}} \|\mathbf{y} - \beta_0 - \mathbf{X}\,\boldsymbol{\beta}\|_2^2 + \alpha\,\|\boldsymbol{\beta}\|_2^2 \tag{10}$$

$$\mathrm{Var}(\hat{\beta}_i) = \mathbb{E}(\hat{\beta}_i - \mathbb{E}(\hat{\beta}_i))^2$$



$$\mathrm{Bias}(\hat{\beta}_i) = \mathbb{E}(\hat{\beta}_i) - \beta_i$$

Setting hyperparameters

How can we choose the ridge hyperparameter α?

Try a few and pick the best one...
But measure its performance on separate data!

Nested cross-validation

When you hear "best", "maximum", "select", . . . think "bias"

Nested cross-validation

When you hear "best", "maximum", "select", ... think "bias"

Setting the parameters

- **Select** β that gives the **best** prediction on training data
- The prediction score for $\hat{\beta}$ is biased: compute a new score on unseen test data.

Nested cross-validation

When you hear "best", "maximum", "select", ... think "bias"

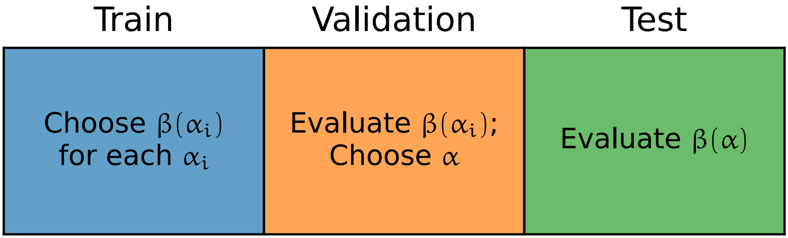
Setting the parameters

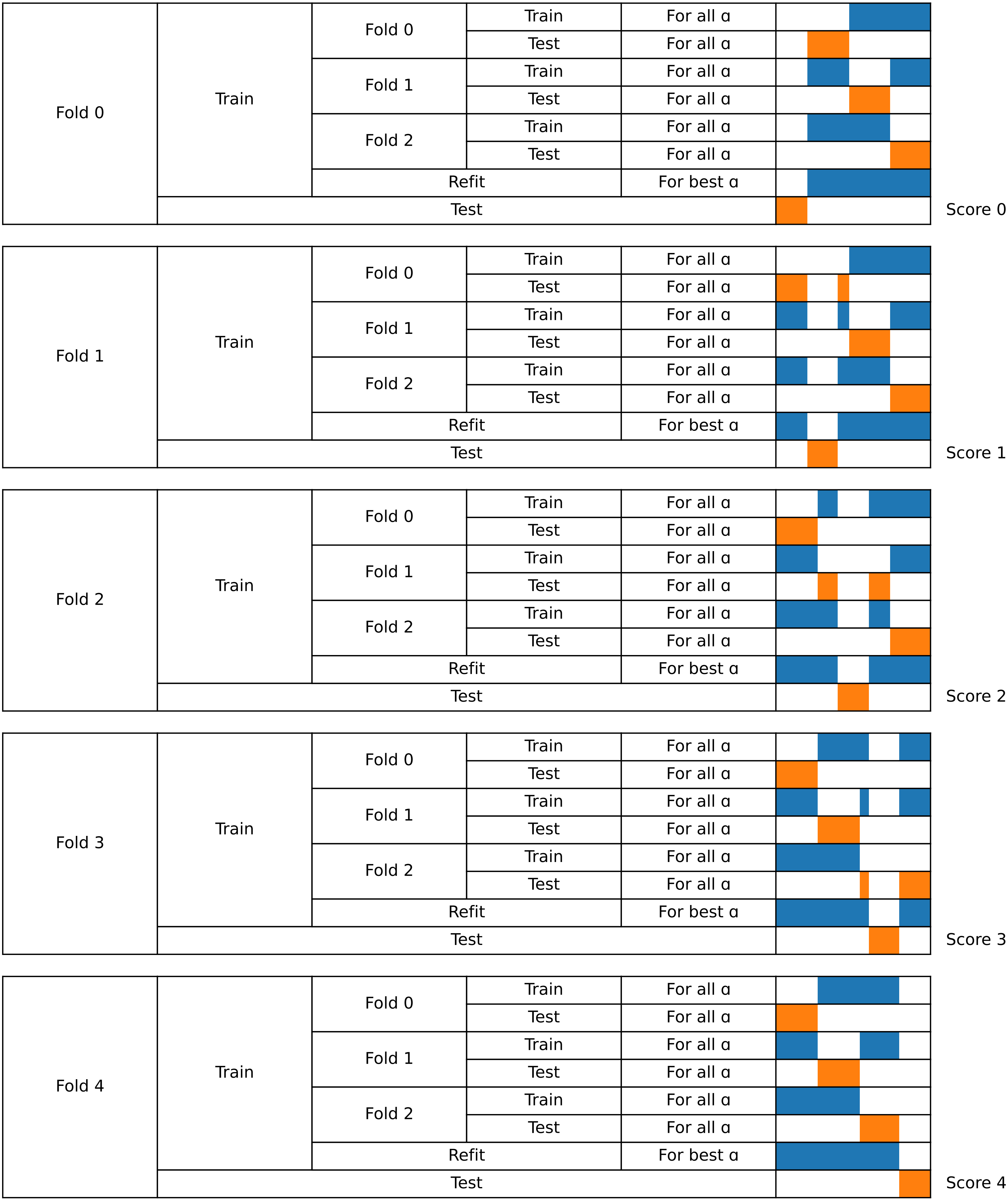
- **Select** β that gives the **best** prediction on training data
- The prediction score for $\hat{\beta}$ is biased: compute a new score on unseen test data.

Setting the hyperparameters

- Repeat step 1 for a few values of α, fitting and testing several models
- **Select** the hyperparameter that obtains the **best** prediction on test data
- The prediction score of that model on *test* data is biased: evaluate it again on unseen data

One split


Train
Validation
Test
Choose $\beta(\alpha_i)$ for each α_i
Evaluate $\beta(\alpha_i)$; Choose α
Evaluate $\beta(\alpha)$


Fold 0
Train
Fold 0
Train
For all α
Test
For all α
Fold 1
Train
For all α
Test
For all α
Fold 2
Train
For all α
Test
For all α
Refit
For best α
Test
Score 0
Fold 1
Train
Fold 0
Train
For all α
Test
For all α
Fold 1
Train
For all α
Test
For all α
Fold 2
Train
For all α
Test
For all α
Refit
For best α
Test
Score 1
Fold 2
Train
Fold 0
Train
For all α
Test
For all α
Fold 1
Train
For all α
Test
For all α
Fold 2
Train
For all α
Test
For all α
Refit
For best α
Test
Score 2
Fold 3
Train
Fold 0
Train
For all α
Test
For all α
Fold 1
Train
For all α
Test
For all α
Fold 2
Train
For all α
Test
For all α
Refit
For best α
Test
Score 3
Fold 4
Train
Fold 0
Train
For all α
Test
For all α
Fold 1
Train
For all α
Test
For all α
Fold 2
Train
For all α
Test
For all α
Refit
For best α
Test
Score 4

Nested cross-validation with scikit-learn

- In general: `GridSearchCV` (User Guide)

```
model = GridSearchCV(
    Ridge(), {"alpha": [.1, 1., 10.]})
scores = cross_val_score(model, X, y)
```

- Use CV estimators when possible: `RidgeCV`, `LassoCV`, . . .

`ex_03_grid_search_regression_questions.py`

Implementing nested CV

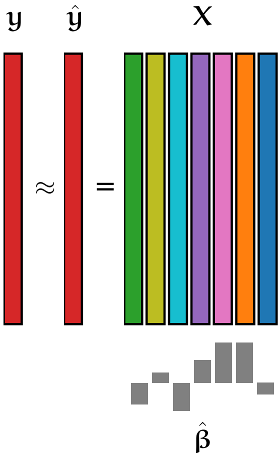
`ex_04_nested_cross_validation_questions.py`

Outline

Dimensionality reduction

Linear regression: projection on the column space of $\mathbf{X}$

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}} \qquad (11)$$

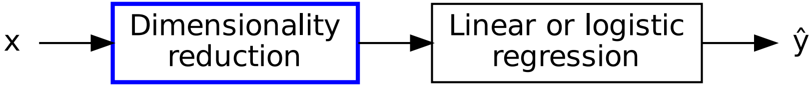


- Too many features: high variance & unstable solution
- Solutions: regularization, **dimensionality reduction**

Dimensionality reduction

Until now

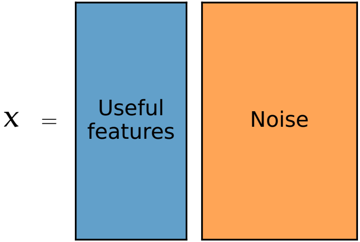
Add a step in the pipeline: simplifying the inputs



Simulated data for linear regression

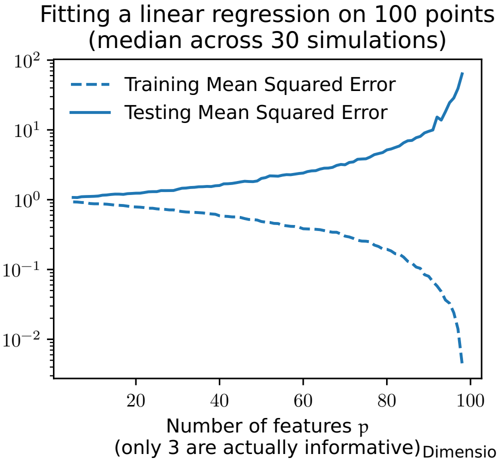
- Generate $\mathbf{X} \in \mathbb{R}^{n \times 3}$, $\boldsymbol{\beta} \in \mathbb{R}^3$, $\boldsymbol{e} \in \mathbb{R}^n$ and $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{e} \in R^n$
- Append columns containing random noise to $\mathbf{X}$
- Now $\mathbf{X} \in \mathbb{R}^{n \times p}$, with $p \geqslant 3$, but only the first 3 columns are linked with $\mathbf{y}$
- Split into training and testing tests and evaluate a linear regression model: what happens when p becomes large?

See `sklearn.datasets.make_regression` for generating data



Model complexity: overfitting

- Model complexity increases with dimension.
- Example: a linear model in dimension p can fit exactly (0 training error) any set of $p + 1$ points.
- Risk of overfitting: fitting exactly training data but failing on test data



Univariate feature selection

- a.k.a. feature screening, filtering ...
- Check features (columns of X) one by one for association with the output y
- Keep only a fixed number or percentage of the features

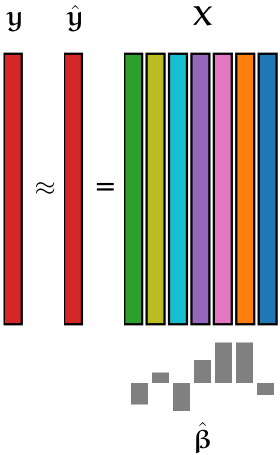
Simple (linear) association criteria

- for regression: correlation
- for classification: ANalysis Of VAriance

Read more in the scikit-learn user guide
scikit-learn feature selection

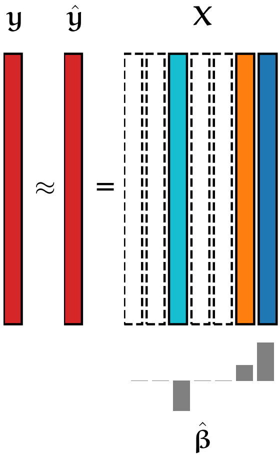
Original regression problem

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}} \qquad (12)$$



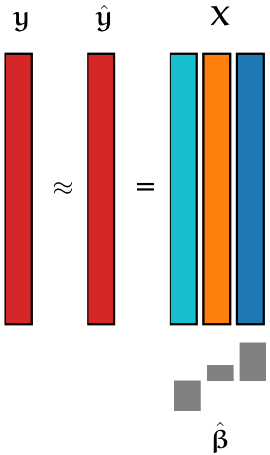
After univariate feature selection

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}} \qquad (13)$$



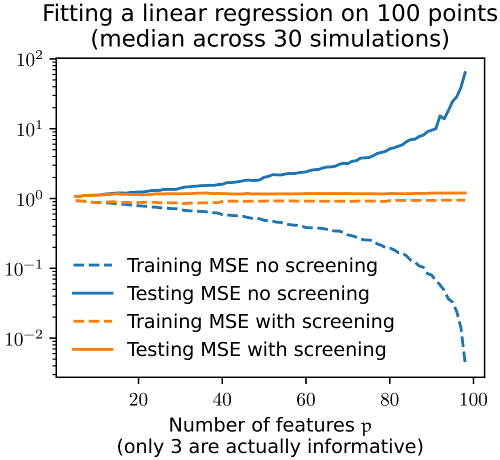
After univariate feature selection

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}} \qquad (14)$$



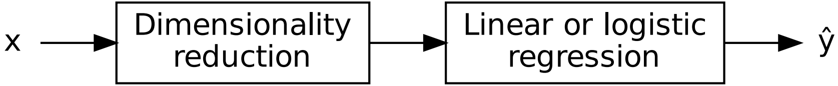
Univariate feature selection

Keeping only the 10 best features (most correlated with y)

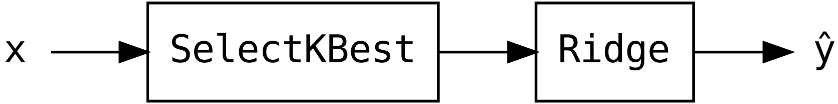


Dataset transformations

Typical pipeline



Example



scikit-learn "transformer API": `fit; transform`

```
transformer = SelectKBest()
transformer.fit(X_train, y_train)
transformed_train = transformer.transform(X_train)
```

can also be written:

```
transformer = SelectKBest()
transformed_train = transformer.fit_transform(
    X_train, y_train)
```

scikit-learn feature selection
scikit-learn Transformer API

`feature_selection.SelectKBest`

`fit:`

- compute ANOVA or correlation for each column of X
- Remember the indices of the k columns with highest scores

`transform:`

- Index input to keep only the k selected columns

`sklearn.feature_selection.SelectKBest`

Fit the transformer only on train data!

```
transformer = SelectKBest()
transformed_train = transformer.fit_transform(
    X_train, y_train)

transformed_test = transformer.transform(X_test)
```

Pipelines

To chain transformations and an estimator, use `sklearn.pipeline.Pipeline`

- can be used to properly cross-validate whole pipeline
- can be combined with `cross_validate`, `GridSearchCV`, ...
- easily created with `sklearn.pipeline.make_pipeline`

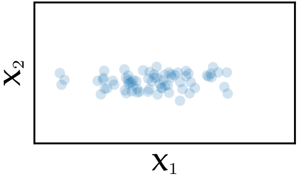
```
model = make_pipeline(SelectKBest(), Ridge())
```

`ex_05_feature_selection_questions.py`

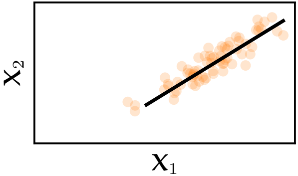
Linear decomposition methods

Another approach to dimensionality reduction

Maybe OK to drop x_2:

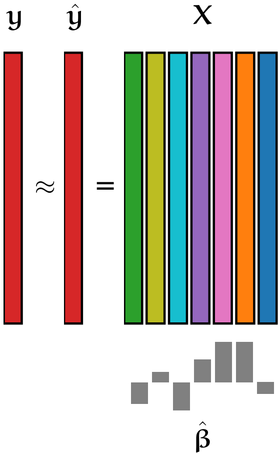


Data low-dimensional but no feature can be dropped:



Find a better referential in which to represent the data

Linear regression: projection on the column space of X



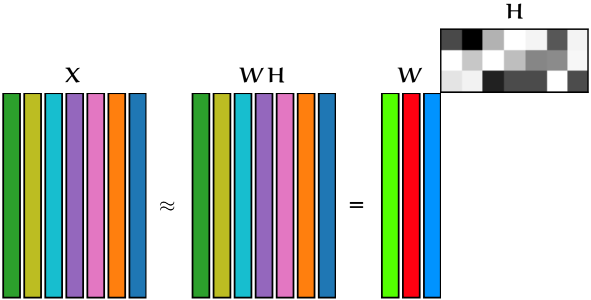
$$\hat{y} = X\,\hat{\beta} \qquad (15)$$

- Too many features: high variance & unstable solution
- Feature selection: drop some columns of X
- Other ways to build a family of k vectors on which to regress y?

Linear decomposition: low-rank approximation of X

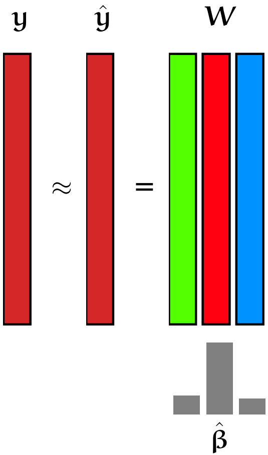
Minimize

$$\|X - WH\|_F^2 = \sum_{i,j} (X_{i,j} - (WH)_{i,j})^2 \tag{16}$$



Linear regression after dimensionality reduction

$$\hat{\mathbf{y}} = \mathbf{W}\,\hat{\boldsymbol{\beta}} \tag{17}$$



Prediction for a new data point $x \in \mathbb{R}^p$

- Find the combination of rows of H that is closest to x: regress x on H^T
- Multiply by $\hat{\beta}$

$$x \in \mathbb{R}^p \to \text{projection} \to w \in \mathbb{R}^k \to \langle \cdot\, , \hat{\beta} \rangle \to \hat{y} \in \mathbb{R} \tag{18}$$

Principal Component Analysis

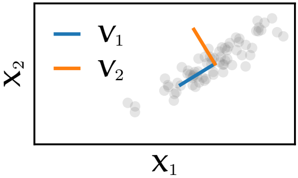
- Singular Value Decomposition of $\mathbf{X}$:

$$\mathbf{X} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}} \tag{19}$$

with $\mathbf{X} \in \mathbb{R}^{n \times p}$, $\mathbf{U} \in \mathbb{R}^{n \times r}$, $\mathbf{S} \in \mathbb{R}^{r \times r}$, $\mathbf{V} \in \mathbb{R}^{r \times p}$

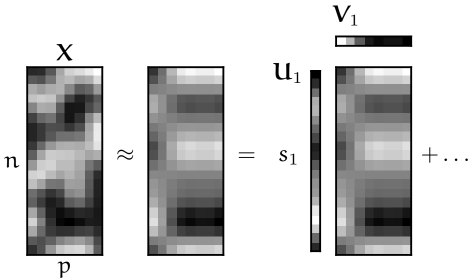
- $r = \min(n, p)$
- $\mathbf{S} \succeq 0$ diagonal with decreasing values s_j along the diagonal
- $\mathbf{U}^{\mathsf{T}}\,\mathbf{U} = I_r$
- $\mathbf{V}^{\mathsf{T}}\,\mathbf{V} = I_r$

Truncating the SVD to keep only the first k components gives the best rank-k approximation of $\mathbf{X}$



Singular Value Decomposition

$$X = U S V^{\mathsf{T}} \tag{20}$$



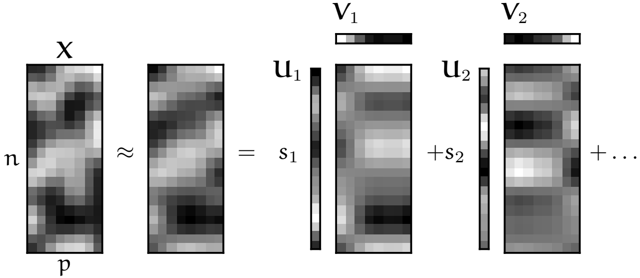
Explained variance: 0.53

$$U^{\mathsf{T}} U = I_p \tag{21}$$

$$V^{\mathsf{T}} V = I_p \tag{22}$$

Singular Value Decomposition

$$X = U S V^{\mathsf{T}} \tag{23}$$



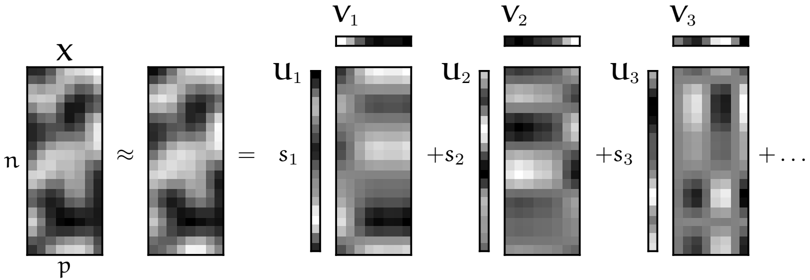
Explained variance: 0.84

$$U^{\mathsf{T}} U = I_p \tag{24}$$

$$V^{\mathsf{T}} V = I_p \tag{25}$$

Singular Value Decomposition

$$X = U\,S\,V^T \tag{26}$$



Explained variance: 0.97

$$U^T\,U = I_p \tag{27}$$

$$V^T\,V = I_p \tag{28}$$

Other decomposition methods

Many other methods use the same objective (sum of squared reconstruction errors), but add penalties or constraints on the factors

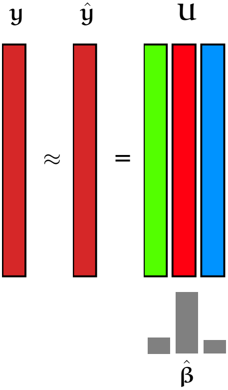
- Dictionary Learning
- Non-negative Matrix Factorization
- K-means clustering
- ...

What about $\mathfrak{y}$?

- PCA is an example of *unsupervised* learning: it does not use $\mathfrak{y}$
- Some other methods take it into account: e.g. Partial Least Squares

Ridge regression and PCA

- Both ridge regression and PC regression compute the coordinates of y in the basis given by the SVD of X
- Ridge shrinks the coordinate along u_j by a factor $s_j^2/(s_j^2+\alpha)$
- PC regression sets the coordinates to 0 except for those corresponding to the k largest s_j: shrinks by a factor $1_{\{j \leqslant k\}}$



Outline

(Cross-)validation experiments are simulations

The validation experiments must simulate what will happen when deploying the trained model in production – when starting to use it in real life.

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Example (Deploying a model to a hospital)

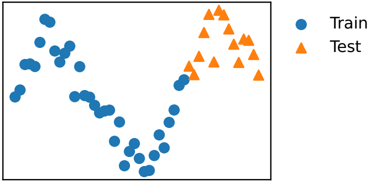
A model is trained on research dataset and then shipped and used on a hospital's patients. We cannot:

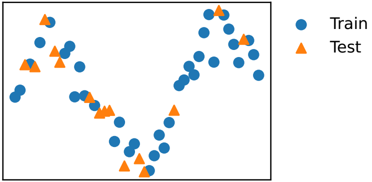
- Preprocess the patients' data together with the training data.
- Use the patients' data for feature selection.
- Try different models on the patients' data and pick the best.

If we do any of these things in our cross-validation it is not a realistic experiment.

Split choice example: time series

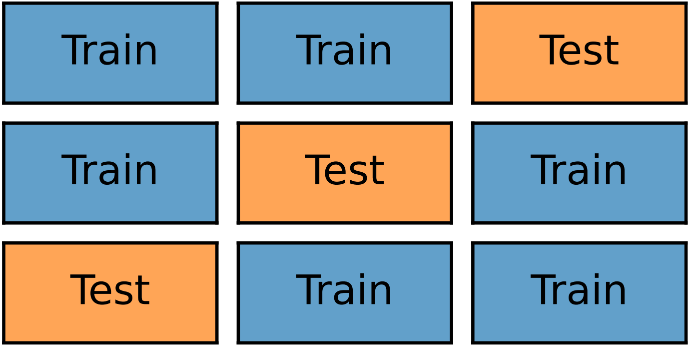
Don't ignore dependencies between samples: which is easier?





Use the appropriate cross-validation iterator

Remember that CV training sets overlap



So the scores are not independent! Their variance can be underestimated.

Some pitfalls with cross-validation

Overfitting the hyperparameters

- select hyperparameters with nested CV `sklearn.model_selection.GridSearchCV`

Fitting part of the pipeline on the whole dataset

- use `sklearn.pipeline.Pipeline`

Ignoring dependencies between samples

- e.g. time series: use appropriate cross-validation iterator

Ignoring dependencies between CV scores

- Training sets overlap: cross-validation scores of different splits are not independent

Over-interpreting good CV scores