

# Model selection and validation

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MAIN educational 2022-12-10



# Outline

Introduction: cross-validation

Model and hyperparameter selection

Dimensionality reduction

Conclusion: summary of pitfalls

# Setup reminder

## Clone the repository

```
git clone --depth 1 \
  git@github.com:neurodatascience/main-edu-courses-ml.git
cd main-edu-courses-ml/ml_model_selection_and_validation
evince model_selection_and_validation.pdf &
cd exercises
```

## Install Python and required packages

```
pip install -U -r requirements.txt
```

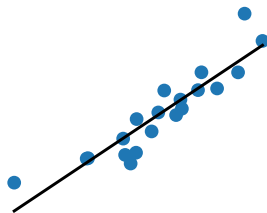
- repository:  
[github.com/neurodatascience/main-edu-courses-ml](https://github.com/neurodatascience/main-edu-courses-ml)
- [notebooks in google drive](#)

# Recap of part 1

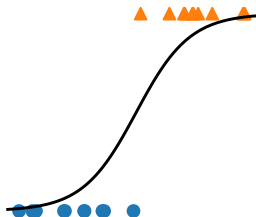
## Supervised learning

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

Linear regression



Logistic regression



# Recap of part 1

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## Regularization

- $\ell_2$  a.k.a. ridge regularization

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## Supervised learning

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

## Regularization

- $\ell_2$  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

$$Y = f(X) + E \quad (1)$$

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

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- $X \in \mathbb{R}^p$ : features (a.k.a. inputs, regressors, descriptors, independent variables)
- $E \in \mathbb{R}$ : unmodelled noise

# Notation & vocabulary

## Supervised learning framework

$$Y = f(X) + E \quad (1)$$

- $Y \in \mathbb{R}$ : output (a.k.a. target, dependent variable) to predict
- $X \in \mathbb{R}^p$ : features (a.k.a. inputs, regressors, descriptors, independent variables)
- $E \in \mathbb{R}$ : unmodelled noise
- $f$ : the function we try to approximate

## Example (Linear regression)

$$Y = \beta_0 + \langle X, \beta \rangle + E \quad (2)$$

$$= \beta_0 + \sum_{j=1}^p X_j \beta_j + E \quad (3)$$

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

# 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  $\mathbf{X} \in \mathbb{R}^{n \times p}$ ,  $\mathbf{y} \in \mathbb{R}^n$ , minimize the empirical risk:  $\sum_{i=1}^n L(\mathbf{y}_i, \hat{\mathbf{y}}_i)$

For linear regression:

find  $\hat{\beta}_0 \in \mathbb{R}$ ,  $\hat{\beta} \in \mathbb{R}^p$  that minimize

$$\|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \|\mathbf{y} - \hat{\beta}_0 - \mathbf{X} \hat{\beta}\|_2^2 \quad (4)$$

$$= \sum_{i=1}^n (\mathbf{y}_i - \hat{\beta}_0 - \sum_{j=1}^p \mathbf{x}_{ij} \hat{\beta}_j)^2 \quad (5)$$

"Fitting" the parameters to  $\mathbf{X}, \mathbf{y}$ .

# Evaluating a model

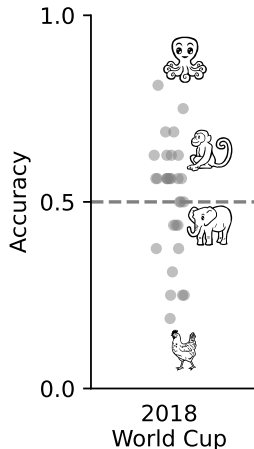
We always want to do 2 distinct things:

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

We can never do both on the same data!

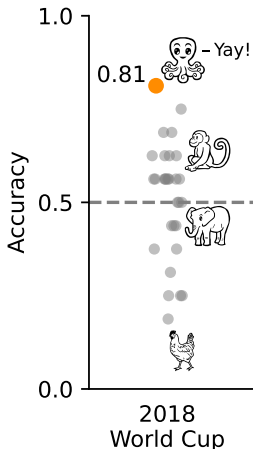
# Training error is a biased estimator of the risk

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



# Training error is a biased estimator of the risk

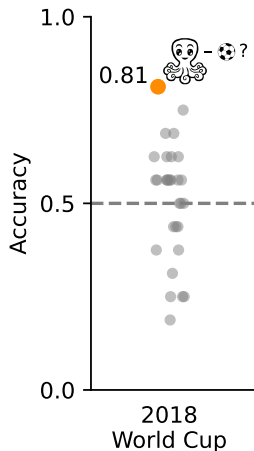
- 30 different animals made predictions about match results in the 2018 world cup
- We **selected the best predictor** (highest accuracy)



# 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:

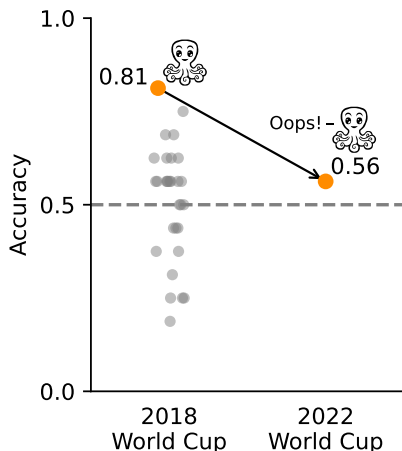
1. Better than in 2018?
2. Worse than in 2018?
3. The same?



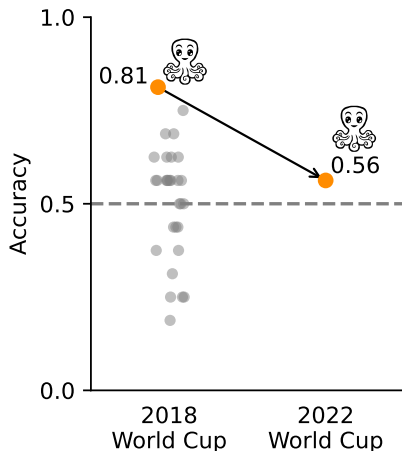


# Training error is a biased estimator of the risk

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



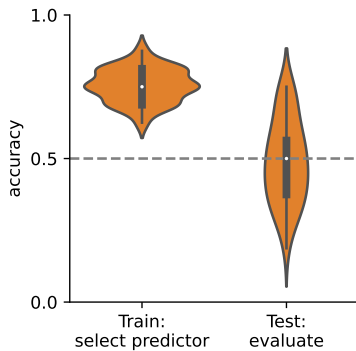
Training error is a biased estimator of the risk  
The selected animal is more likely to perform **worse** than in 2018.



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

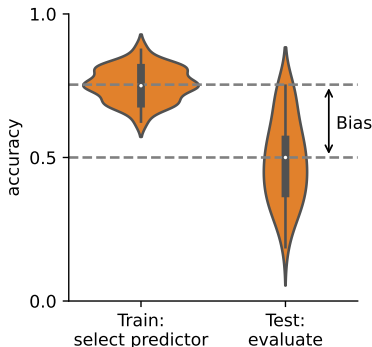
# Training error is a biased estimator of the risk

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**  $\beta$  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`

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

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

Mean Squared Error (MSE): `mean_squared_error`











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

Mean Absolute Error (MAE): `mean_absolute_error`

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



# Cross-validation

Fold 0	Train		Score 0
	Test		
Fold 1	Train		Score 1
	Test		
Fold 2	Train		Score 2
	Test		
Fold 3	Train		Score 3
	Test		
Fold 4	Train		Score 4
	Test		

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**

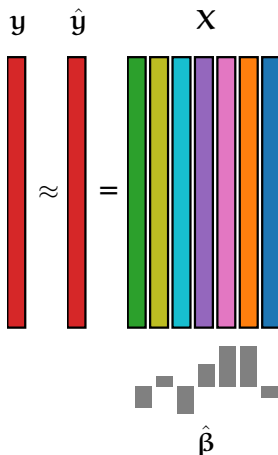
Dimensionality reduction

Conclusion: summary of pitfalls

# Need for regularization

Linear regression: projection on the column space of  $X$

$$\hat{y} = X \hat{\beta} \quad (9)$$

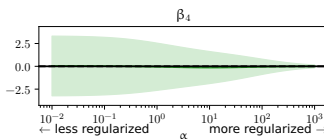
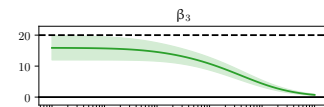
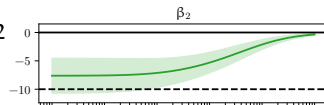
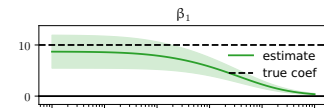
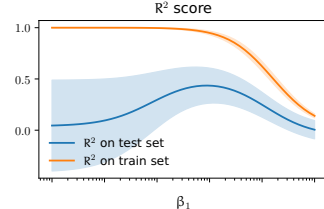


- Too many features: high variance & unstable solution
- Solutions: **regularization**, dimensionality reduction

# Regularization

## Example (Ridge regression)

$$\operatorname{argmin}_{\boldsymbol{\beta}, \beta_0} \|\mathbf{y} - \beta_0 - \mathbf{X} \boldsymbol{\beta}\|_2^2 + \alpha \|\boldsymbol{\beta}\|_2^2 \quad (10)$$



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

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

# Setting hyperparameters

How can we choose the ridge hyperparameter  $\alpha$ ?

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**  $\beta$  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**  $\beta$  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  $\alpha$ , 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

Fold 0	Train	Fold 0	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Fold 1	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Fold 2	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Refit			For best $\alpha$	
		Test				

Fold 1	Train	Fold 0	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Fold 1	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Fold 2	Train	For all $\alpha$		
			Test	For all $\alpha$		
		Refit		For best $\alpha$		
	Test					

Fold 2	Train	Fold 0	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Fold 1	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Fold 2	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Refit		For best $\alpha$			
	Test						

Fold 3	Train	Fold 0	Train	For all $\alpha$				
			Test	For all $\alpha$				
		Fold 1	Train	For all $\alpha$				
			Test	For all $\alpha$				
		Fold 2	Train	For all $\alpha$				
			Test	For all $\alpha$				
		Refit		For best $\alpha$				
	Test							

Fold 4	Train	Fold 0	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Fold 1	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Fold 2	Train	For all $\alpha$			
			Test	For all $\alpha$			
		Refit		For best $\alpha$			
	Test						

# Nested cross-validation

Fold 0	Train	Fold 0	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 1	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 2	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Refit		For best $\alpha$	
	Test				
				Score 0	

Fold 1	Train	Fold 0	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 1	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 2	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Refit		For best $\alpha$	
	Test				
Score 1					

Fold 2	Train	Fold 0	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 1	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 2	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Refit		For best $\alpha$	
	Test				
Score 2					

Fold 3	Train	Fold 0	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 1	Train	For all $\alpha$	
			Test	For all $\alpha$	
		Fold 2	Train	Model and hyperparameter	
			Test	For all $\alpha$	

# 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

Introduction: cross-validation

Model and hyperparameter selection

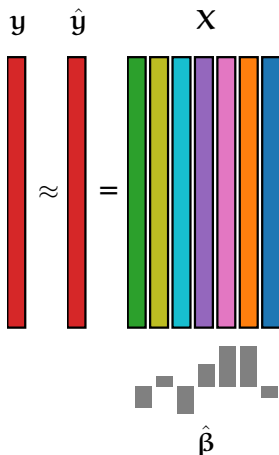
**Dimensionality reduction**

Conclusion: summary of pitfalls

# Dimensionality reduction

Linear regression: projection on the column space of  $X$

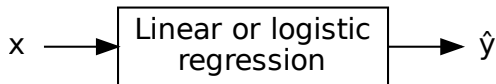
$$\hat{y} = X\hat{\beta} \quad (11)$$



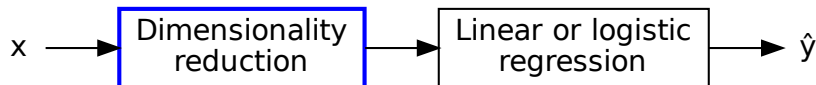
- Too many features: high variance & unstable solution
- Solutions: regularization, **dimensionality reduction**

# Dimensionality reduction

Until now



Add a step in the pipeline: simplifying the inputs

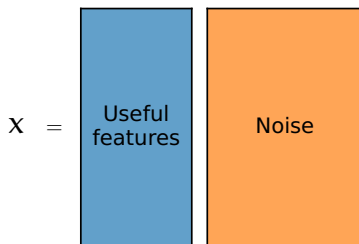




# Simulated data for linear regression

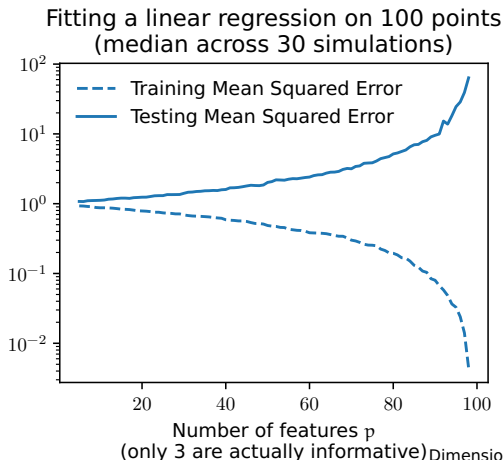
- Generate  $\mathbf{X} \in \mathbb{R}^{n \times 3}$ ,  $\boldsymbol{\beta} \in \mathbb{R}^3$ ,  $\mathbf{e} \in \mathbb{R}^n$  and  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} \in \mathbb{R}^n$
- Append columns containing random noise to  $\mathbf{X}$
- Now  $\mathbf{X} \in \mathbb{R}^{n \times p}$ , with  $p \geq 3$ , 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

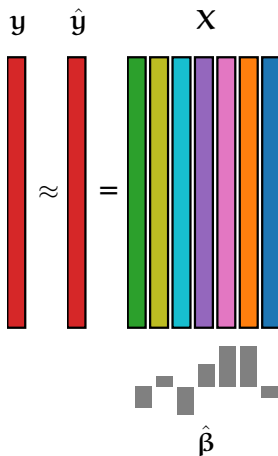
## Simple (linear) association criteria

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

Read more in the scikit-learn user guide  
[scikit-learn feature selection](#)

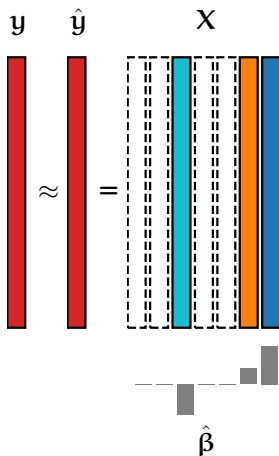
# Original regression problem

$$\hat{y} = X\hat{\beta} \quad (12)$$



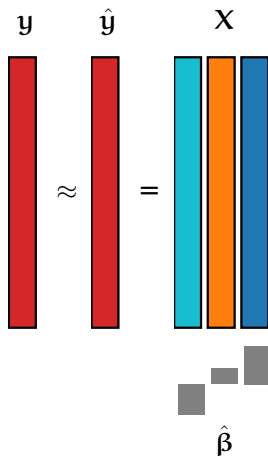
# After univariate feature selection

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



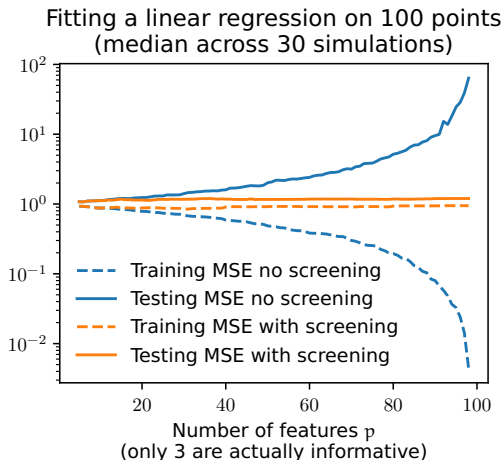
# After univariate feature selection

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



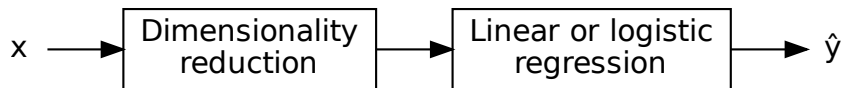
# Univariate feature selection

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`

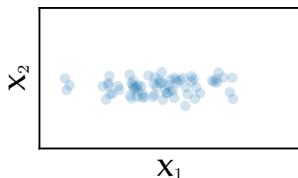
```
model = make_pipeline(SelectKBest(), Ridge())
```

`ex_05_feature_selection_questions.py`

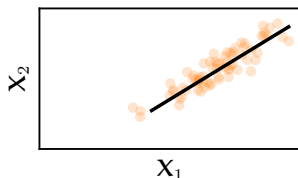
# Linear decomposition methods

Another approach to dimensionality reduction

Maybe OK to drop  $X_2$ :



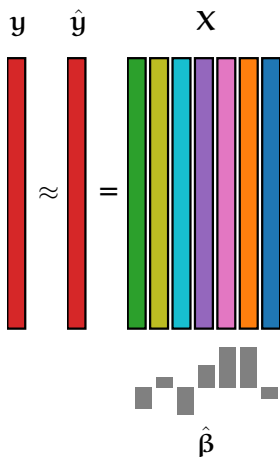
Data low-dimensional but no feature can be dropped:



Find a better referential in which to represent the data

# Linear regression: projection on the column space of $X$

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

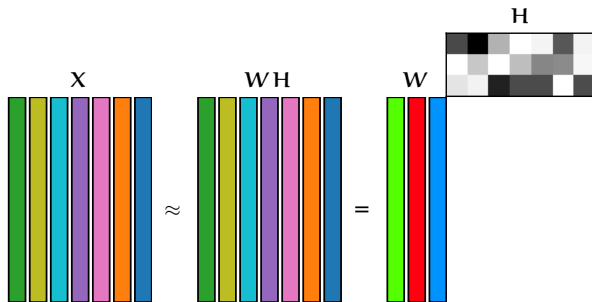


- Too many features: high variance & unstable solution
- Feature selection: drop some columns of  $X$
- Other ways to build a family of  $k$  vectors on which to regress  $y$ ?

# Linear decomposition: low-rank approximation of $X$

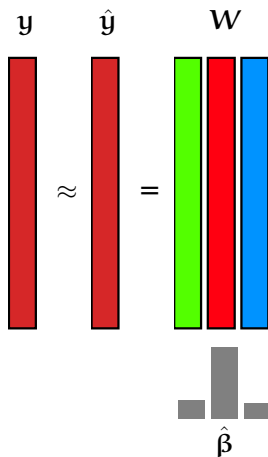
Minimize

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



# Linear regression after dimensionality reduction

$$\hat{y} = W \hat{\beta} \quad (17)$$





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

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

$$\mathbf{x} \in \mathbb{R}^p \rightarrow \text{projection} \rightarrow \mathbf{w} \in \mathbb{R}^k \rightarrow \langle \cdot, \hat{\boldsymbol{\beta}} \rangle \rightarrow \hat{y} \in \mathbb{R} \quad (18)$$

# Principal Component Analysis

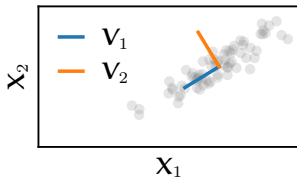
- Singular Value Decomposition of  $X$ :

$$X = U S V^T \quad (19)$$

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

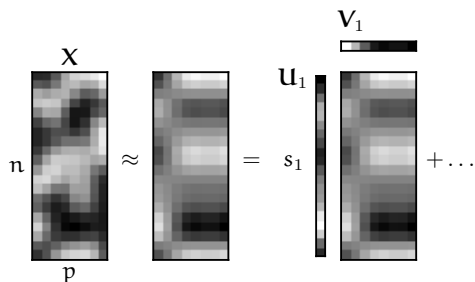
- $r = \min(n, p)$
- $S \succeq 0$  diagonal with decreasing values  $s_j$  along the diagonal
- $U^T U = I_r$
- $V^T V = I_r$

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



# Singular Value Decomposition

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^T \quad (20)$$



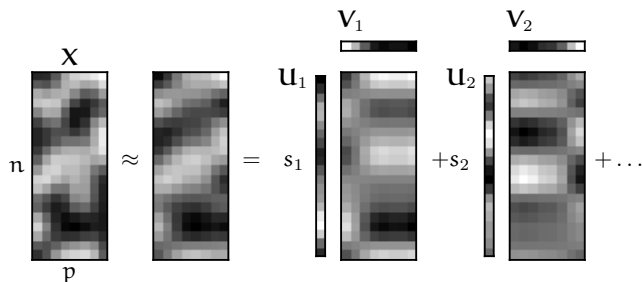
Explained variance: 0.53

$$\mathbf{U}^T \mathbf{U} = \mathbf{I}_p \quad (21)$$

$$\mathbf{V}^T \mathbf{V} = \mathbf{I}_p \quad (22)$$

# Singular Value Decomposition

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^T \quad (23)$$



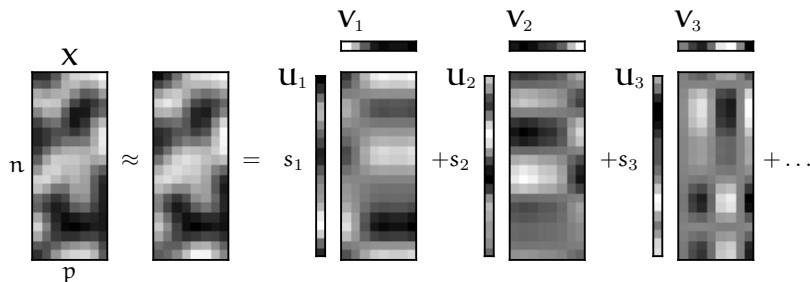
Explained variance: 0.84

$$\mathbf{U}^T \mathbf{U} = \mathbf{I}_p \quad (24)$$

$$\mathbf{V}^T \mathbf{V} = \mathbf{I}_p \quad (25)$$

# Singular Value Decomposition

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^T \quad (26)$$



Explained variance: 0.97

$$\mathbf{U}^T \mathbf{U} = \mathbf{I}_p \quad (27)$$

$$\mathbf{V}^T \mathbf{V} = \mathbf{I}_p \quad (28)$$

# Other decomposition methods

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

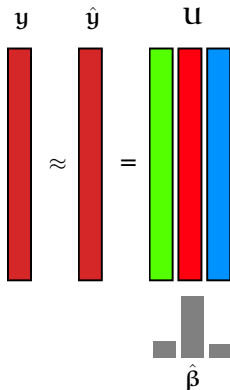
- Dictionary Learning
- Non-negative Matrix Factorization
- K-means clustering
- ...

What about  $y$ ?

- PCA is an example of *unsupervised* learning: it does not use  $y$
- 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  $1_{\{j \leq k\}}$



# Outline

Introduction: cross-validation

Model and hyperparameter selection

Dimensionality reduction

Conclusion: summary of pitfalls



# (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.

# (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.

## Example (Deploying a model to a hospital)

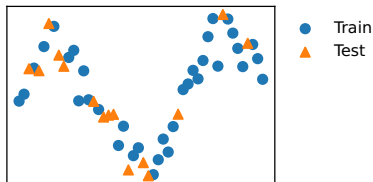
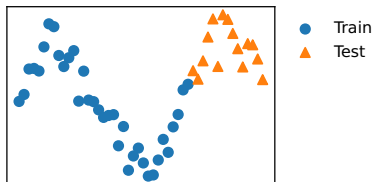
A model is trained on research dataset and then shipped and used on a hospital's patients. We cannot:

- 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.

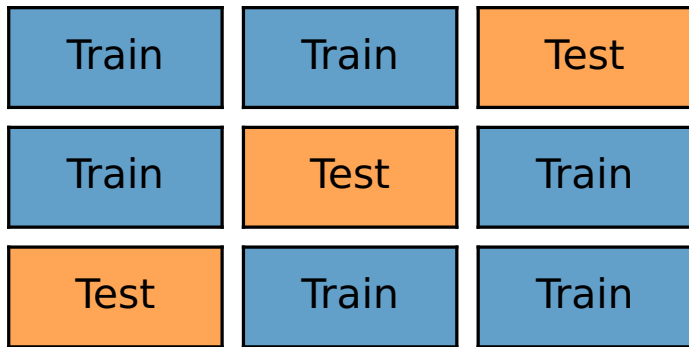
# Split choice example: time series

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