Machine learning Part 2

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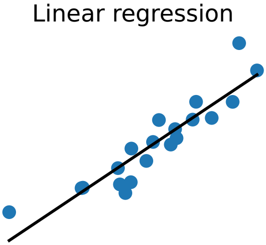
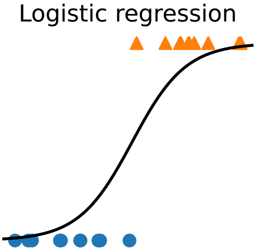
QLS course 2021-07-30

Recap of part 1

Supervised learning

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





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Regularization

- ℓ_2 a.k.a. ridge regularization

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Model evaluation and selection

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

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Don't remember? watch Part 1 again!

Notation & vocabulary
Supervised learning framework

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

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

Example: linear regression

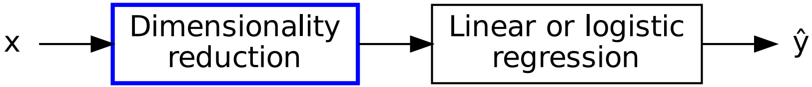
$$\begin{aligned} Y &= \beta_0 + \langle X, \beta \rangle + E & (2) \\ &= \beta_0 + \sum_{j=1}^{p} X_j \, \beta_j + E & (3) \end{aligned}$$

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

Dimensionality reduction

Until now

Add a step in the pipeline: simplifying the inputs



Dimensionality reduction

Problems when the number of features p becomes large

- Bigger errors on test data (larger variance of predictions)
- Numerical stability issues
- Computational cost and memory usage

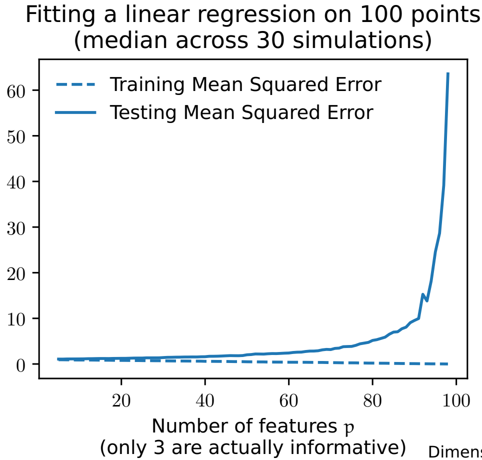
Toy example: linear regression with simulated data

- Generate $\mathbf{X} \in \mathbb{R}^{n \times 3}$, $\boldsymbol{\beta} \in \mathbb{R}^3$, and $\mathbf{y} = \mathbf{X}\,\boldsymbol{\beta} \in R^n$
- 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

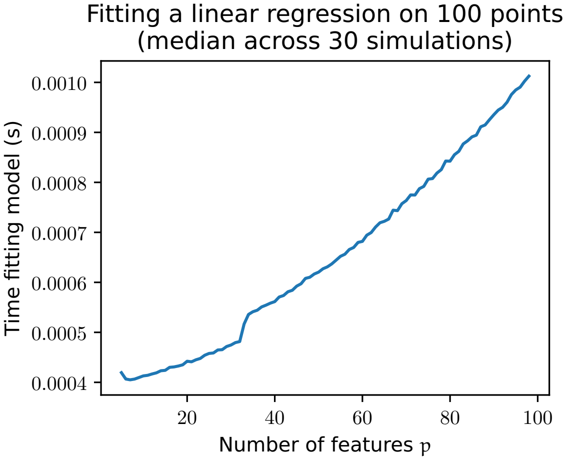
Model complexity: overfitting

- 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



Cost of fitting many parameters

- Many algorithms require polynomial time in p
- Implementations often make copies of the design matrix (e.g. for centering & rescaling)



Univariate feature selection

- a.k.a. feature screening, filtering ...
- Check features (columns of X) one by one for association with the output y
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Simple (linear) association criteria

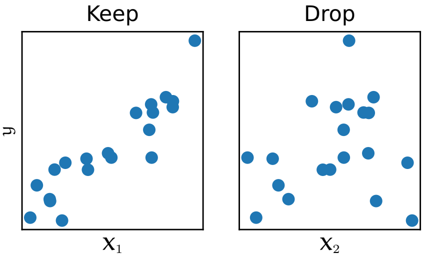
- for regression: correlation
- for classification: ANalysis Of VAriance

Read more in the scikit-learn user guide

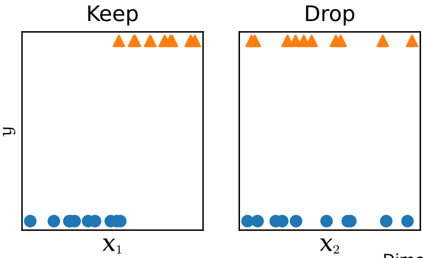
https://scikit-learn.org/stable/modules/feature_selection.html#feature-selection

Simple selection criteria

- Regression: correlation



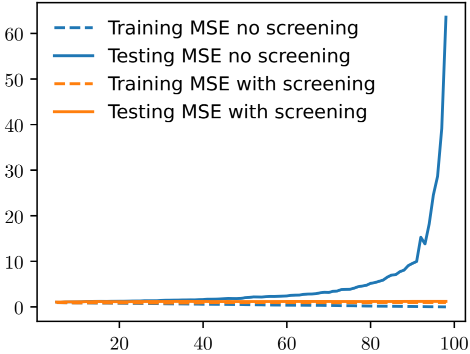
- Classification: ANOVA



Univariate feature selection

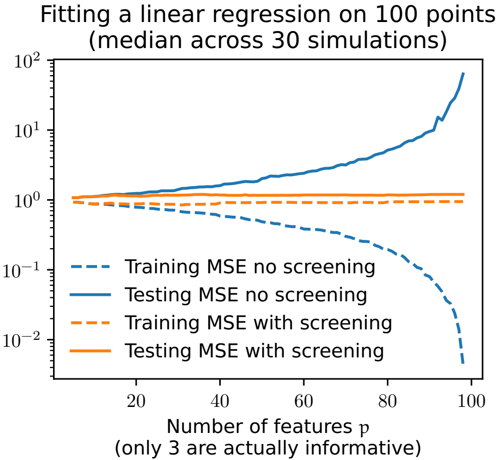
Keeping only the 10 best features (most correlated with y)

Fitting a linear regression on 100 points
(median across 30 simulations)



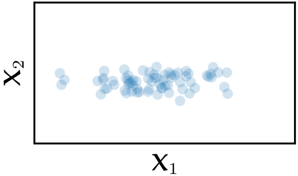
Number of features p
(only 3 are actually informative)

Same plot in log scale

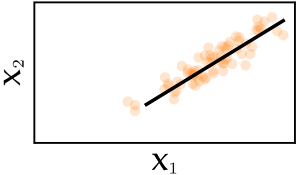


Linear decomposition methods

Maybe OK to drop x_2:



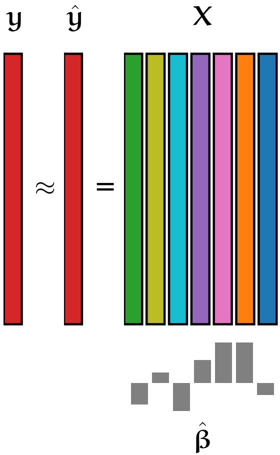
Data low-dimensional but no feature can be dropped:



Find a better referential in which to represent the data

Linear regression: projection on the column space of X

$$\hat{y} = X\hat{\beta} \qquad (4)$$

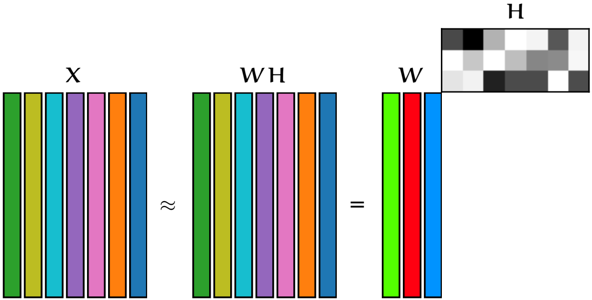


- Too many features: high variance & unstable solution
- Feature selection: drop some columns of X
- Other ways to build a family of k vectors on which to regress y?

Linear decomposition: low-rank approximation of X

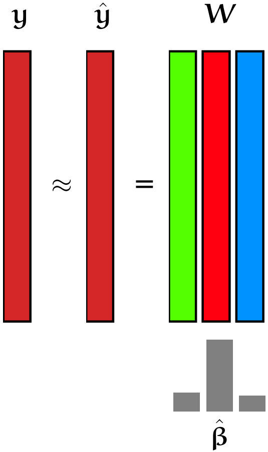
Minimize

$$\|X - WH\|_F^2 = \sum_{i,j} (X_{i,j} - (WH)_{i,j})^2 \quad (5)$$



Linear regression after dimensionality reduction

$$\hat{y} = W\hat{\beta} \quad (6)$$



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 $\hat{\beta}$

$$x \in \mathbb{R}^p \to \text{projection} \to \boldsymbol{w} \in \mathbb{R}^k \to \langle \cdot \, , \, \hat{\boldsymbol{\beta}} \rangle \to \hat{y} \in \mathbb{R} \tag{7}$$

Principal Component Analysis

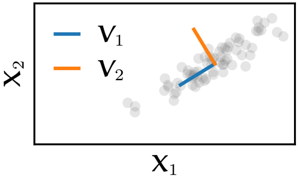
- Singular Value Decomposition of $\mathbf{X}$:

$$\mathbf{X} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\top} \tag{8}$$

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

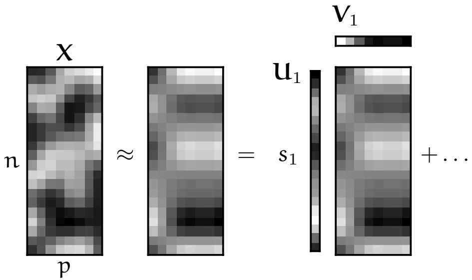
- $r = \min(n, p)$
- $\mathbf{S} \succeq 0$ diagonal with decreasing values s_j along the diagonal
- $\mathbf{U}^{\top}\mathbf{U} = I_r$
- $\mathbf{V}^{\top}\mathbf{V} = I_r$

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



Singular Value Decomposition

$$X = U\,S\,V^T \tag{9}$$



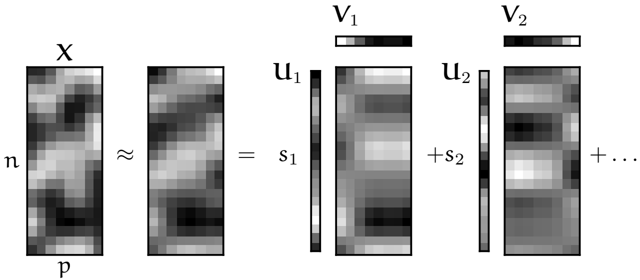
Explained variance: 0.53

$$U^T\,U = I_p \tag{10}$$

$$V^T\,V = I_p \tag{11}$$

Singular Value Decomposition

$$\mathbf{X} = \mathbf{U}\, \mathcal{S}\, \mathbf{V}^{\mathsf{T}} \tag{12}$$



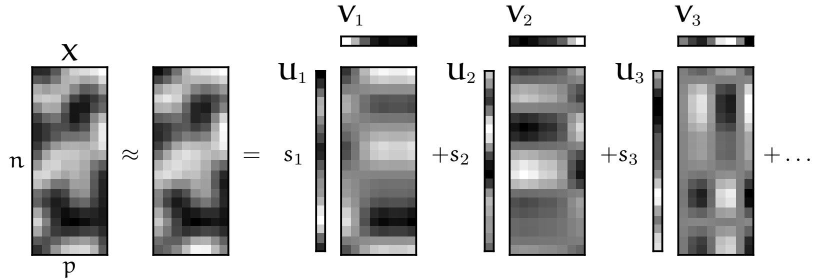
Explained variance: 0.84

$$\mathbf{U}^{\mathsf{T}}\, \mathbf{U} = I_p \tag{13}$$

$$\mathbf{V}^{\mathsf{T}}\, \mathbf{V} = I_p \tag{14}$$

Singular Value Decomposition

$$X = U\,S\,V^{\top} \tag{15}$$



Explained variance: 0.97

$$U^{\top}U = I_p \tag{16}$$

$$V^{\top}V = I_p \tag{17}$$

Other decomposition methods

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

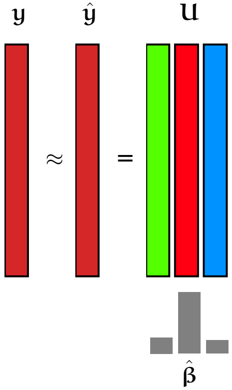
- Dictionary Learning
- Non-negative Matrix Factorization
- K-means clustering
- ...

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 $s_j^2/(s_j^2+\lambda)$
- PC regression sets the coordinates to 0 except for those corresponding to the k largest s_j: shrinks by a factor $1_{\{j \leqslant k\}}$



Setting hyperparameters

How can we choose:

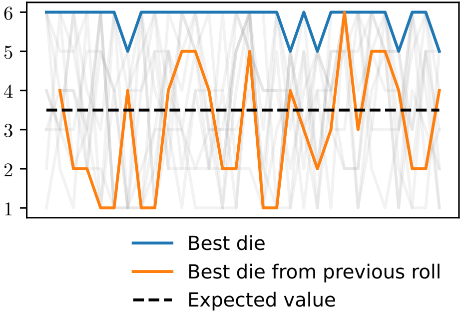
- Number of features or PCA components k?
- The ridge hyperparameter λ?

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

Need for fresh test data

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

- I have 4 dice and want to find one that rolls high numbers
- I roll them all once and select the die that gives the highest number
- The selected die rolled a 5. Is 5 a good estimate of that die's average result? What if I had 1,000 dice?
- I need to roll it again to get an unbiased estimate



Nested cross-validation

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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.

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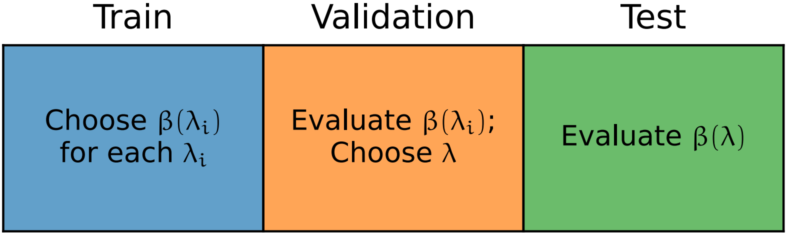
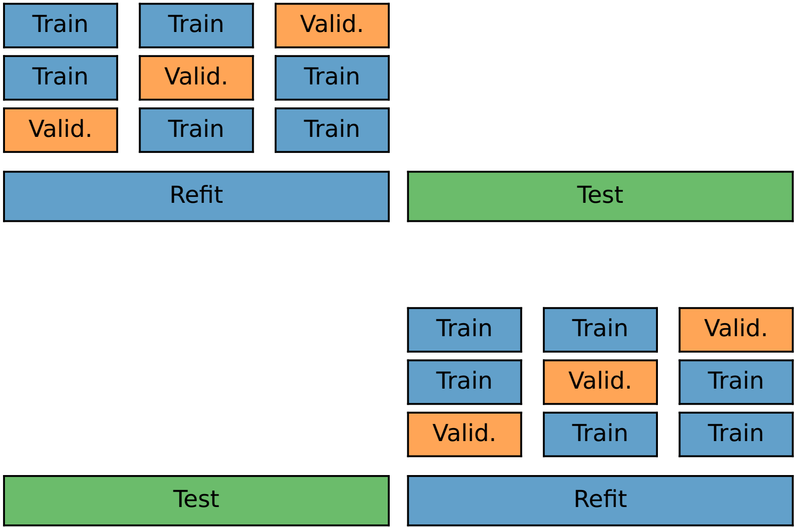
Setting the hyperparameters

- Repeat step 1 for a few values of λ, k, *etc.* ., 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 $\beta(\lambda_i)$ for each λ_i
Evaluate $\beta(\lambda_i)$; Choose λ
Evaluate $\beta(\lambda)$

Nested cross-validation



see `sklearn.model_selection.GridSearchCV`

Some common pitfalls with cross-validation

Fitting part of the pipeline on the whole dataset

- e.g. fit PCA on all data, then do cross-validation on dim-reduced dataset
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- Multiple datapoints per participant
- Time series

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Over-interpreting good CV scores

- Good CV scores on one dataset do not mean the model will always perform well on a new dataset

Supervised learning with fMRI

- Predict in which site / with which scanner a resting-state fMRI sequence was acquired

The decoding pipeline

- Masking: extracting voxels that are inside the brain
- Connectivity: measuring correlations between brain regions to build a feature vector for each participant
- Univariate feature selection with ANalysis Of VAriance
- Classifier: logistic regression

Implementation: in class