SD-TSIA204 - Statistics: linear models
Ridge

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Problems of OLS and Motivation for Ridge Regression

We saw in the first session that $\hat{\theta} = (X^T X)^{-1} X^T Y$ is only well-defined if $(X^T X)^{-1}$ exists.
Collinearity: When two columns of the design matrix $X \in \mathbb{R}^{n \times p}$ are (almost) linearly dependent, $X^T X$ is ill-conditioned.
Supercollinearity: When $n < p$, rank$(X) = \min(n, p) = n$.

Two Approaches:

1. The first uses the Moore-Penrose inverse of the matrix.
2. The second is ridge regression, an ad-hoc fix for inversion problems with an interpretation in terms of penalization of the coefficients.

Method 1, based on the Moore-Penrose inverse

$X^T X\boldsymbol{\theta} = X^T Y$. The matrix $X^T X$ is of rank n, while $\boldsymbol{\theta}$ is a vector of length p. If $p > n$, the vector $\boldsymbol{\theta}$ cannot be uniquely determined from this system of equations.
Rem Let U be the n-dimensional space spanned by the columns of X, and let V be the $p-n$-dimensional space, the orthogonal complement of U, i.e., $V = U^{\perp}$. Then, $Xv = 0_p$ for all $v \in V$, making V the non-trivial null space of X, $Ker(X)$.
Consequently, as $X^T Xv = X^T 0_p = 0_n$, the solution of the normal equations is:

$$\hat{\boldsymbol{\theta}} = (X^T X)^{+} X^T Y + v \quad \text{for all } v \in V,$$

The Moore-Penrose inverse of the matrix A is defined as follows for a square symmetric matrix:

$$A^{+} = \sum_{j=1}^{p} \frac{1}{s_j} v_j v_j^{\top} \mathbb{I}\{s_j \neq 0\}, \quad \text{where } \nu_j \neq 0 \text{ for } j = 1, 2, \ldots, p.$$

Method 2, Ridge

The ridge regression estimator can be seen as an ad-hoc fix for the singularity of X^TX

$$\hat{\theta}_\lambda = (X^TX + \lambda I_{pp})^{-1}X^TY,$$

for $\lambda > 0$.

Exercise Show that $(X^TX + \lambda I_{pp})$ is invertible

Ridge : penalized definition

$$\boxed{\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = \mathop{\arg\min}_{\boldsymbol{\theta}\in\mathbb{R}^p} \left(\underbrace{\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2}_{\textbf{data fitting}} + \underbrace{\lambda\|\boldsymbol{\theta}\|_2^2}_{\textbf{regularization}} \right)}$$

- Note that the *Ridge* estimator is **unique** for any fixed $\lambda > 0$
- We recover the limiting cases:

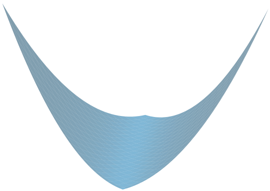
$$\lim_{\lambda\to 0} \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = \hat{\boldsymbol{\theta}}^{\mathrm{OLS}} \text{(solution with smallest } \|\cdot\|_2 \text{ norm)}$$

$$\lim_{\lambda\to +\infty} \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = 0 \in \mathbb{R}^p$$

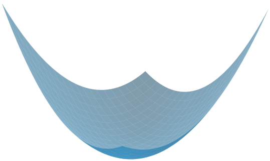
- First order conditions:

$$\nabla f(\boldsymbol{\theta}) = X^\top(X\boldsymbol{\theta} - \mathbf{y}) + \lambda\boldsymbol{\theta} = 0 \Leftrightarrow (X^\top X + \lambda\,\mathrm{Id}_p)\boldsymbol{\theta} = X^\top\mathbf{y}$$

Motivation



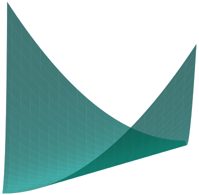
OLS



Ridge

x and y-axis are the OLS coefficients θ_0 and θ_1, z axis is the RSS
Regularize: simplify the problem when ill-conditioned

Motivation



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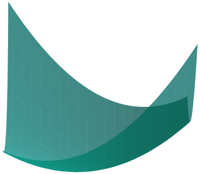

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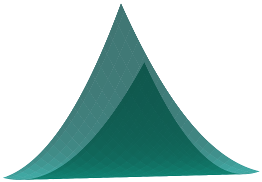

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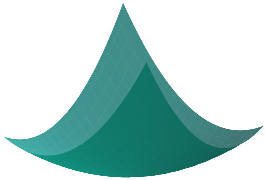

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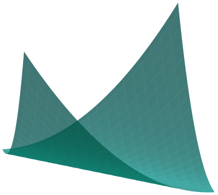

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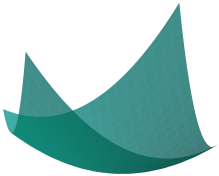

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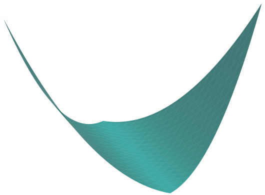

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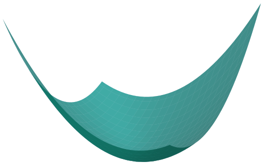


Ridge

x and y-axis are the OLS coefficients θ_0 and θ_1, z axis is the RSS
Regularize: simplify the problem when ill-conditioned

Constraint interpretation

A "Lagrangian" formulation is as follows:

$$\mathop{\arg\min}_{\boldsymbol{\theta}\in\mathbb{R}^p} \left(\underbrace{\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2}_{\textbf{data fitting}} + \underbrace{\lambda\|\boldsymbol{\theta}\|_2^2}_{\textbf{regularization}} \right)$$

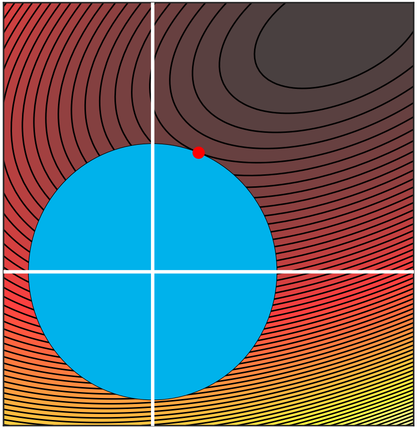
has for a certain $T > 0$ the same solution as:

$$\begin{cases} \mathop{\arg\min}_{\boldsymbol{\theta}\in\mathbb{R}^p} \|\mathbf{y} - X\boldsymbol{\theta}\|_2^2 \\ \text{s.t. } \|\boldsymbol{\theta}\|_2^2 \leqslant T \end{cases}$$

Rem the link $T \leftrightarrow \lambda$ is not explicit!

- If $T \to 0$ we recover the null vector: $0 \in \mathbb{R}^p$
- If $T \to \infty$ we recover $\hat{\boldsymbol{\theta}}^{\mathrm{OLS}}$ (un-constrained)

Level lines and constraint set



Optimization under ℓ_2 constraints:

$$\begin{cases} \underset{\boldsymbol{\theta}\in\mathbb{R}^p}{\arg\min} \|\mathbf{y} - X\boldsymbol{\theta}\|_2^2, \\ \text{s.t. } \|\boldsymbol{\theta}\|_2^2 \leqslant T \end{cases}$$

Associated prediction

From the *Ridge* coefficient:

$$\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = (\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \mathbf{y}$$

the associated prediction is given by:

$$\hat{\mathbf{y}}_\lambda = X \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = X(\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \mathbf{y} = H_\lambda \mathbf{y}$$

Rem the estimator $\hat{\mathbf{y}}_\lambda$ is linear w.r.t. $\mathbf{y}$

Ridge shrinks the singular values

Note $X = UDV^T = \sum_{i=1}^{\mathrm{rg}(X)} s_i \mathbf{u}_i \mathbf{v}_i^\top$, (SVD)
Proposition The ridge penalty shrinks the singular values. To see this, show that $\hat{\theta} = V(D^\top D)^{-1} D^\top U^\top Y$ and $\hat{\theta}_\lambda = V(D^\top D + \lambda I)^{-1} D^\top U^\top Y$

The matrix $H_\lambda := X(\lambda \, \mathrm{Id}_p + X^\top X)^{-1} X^\top = \sum_{j=1}^{\mathrm{rg}(X)} \frac{s_j^2}{s_j^2 + \lambda} \mathbf{u}_j \mathbf{u}_j^\top$ and $H_+ := X(X^\top X)^+ X^\top$ are the equivalent of the hat matrix for both methods respectively
Exercise Show that H^+ is an orthogonal projector and H_λ is not.
Exercise Show that ridge fit $\hat{\mathbf{y}}_\lambda$ is not orthogonal to the associated ridge residuals $\hat{\epsilon}_\lambda$, defined as $\hat{\epsilon}_\lambda = Y - X\hat{\boldsymbol{\theta}}_\lambda$.

Remarks

Reminder: normalizing the p features the same way is necessary if you want the penalty to be similar for all features:

- center the observation and the features $\Rightarrow$ no coefficient for the constants (hence no constraint on it)
- not centering features $\Rightarrow$ do not put constraint on the constant feature (bias/intercept)

$$\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} = \operatorname*{arg\,min}_{\boldsymbol{\theta} \in \mathbb{R}^p} \|\mathbf{y} - X\boldsymbol{\theta} - \theta_0 \mathbf{1}_n\|_2^2 + \lambda \sum_{j=1}^p \theta_j^2$$

Rem for cross validation one can use $\frac{\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2}{2n}$ rather than $\frac{\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2}{2}$ as the data fitting part

General form of the bias

Under the fixed-design model, $\mathbf{y} = X\boldsymbol{\theta}^\star + \boldsymbol{\varepsilon}$ with $\mathbb{E}(\boldsymbol{\varepsilon}) = 0$:

$$\begin{aligned}
\mathbb{E}(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}) &= \mathbb{E}[(\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \mathbf{y}] \\
&= \mathbb{E}[(\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top X \boldsymbol{\theta}^\star + (\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \boldsymbol{\varepsilon}] \\
&= (\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top X \boldsymbol{\theta}^\star \\
&= \sum_{i=1}^{\mathrm{rg}(X)} \frac{s_i^2}{s_i^2 + \lambda} \mathbf{v}_i \mathbf{v}_i^\top \boldsymbol{\theta}^\star
\end{aligned}$$

Rem one recovers $\mathbb{E}(\hat{\boldsymbol{\theta}}^{\mathrm{OLS}}) \to \sum_{i=1}^{\mathrm{rg}(X)} \mathbf{v}_i \mathbf{v}_i^\top \boldsymbol{\theta}^\star$ when$\lambda \to 0$

Exercise Show that the bias for an orthonormal X is $(1 + \lambda)^{-1}\boldsymbol{\theta} - \boldsymbol{\theta}$

Variance in the general case

Under the assumption $\mathbb{E}(\boldsymbol{\varepsilon}) = 0$, and with a homoscedastic model: $\mathbb{E}(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top) = \sigma^2 \operatorname{Id}_n$

Variance / Covariance

$$V_\lambda^{\mathrm{rdg}} = \mathbb{E}\left((\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \mathbb{E}(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}))(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \mathbb{E}(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}})^\top\right)$$

Explicit computation:

$$\begin{aligned} V_\lambda^{\mathrm{rdg}} =& \mathbb{E}((\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top X (\lambda \operatorname{Id}_p + X^\top X)^{-1}) \\ &= (\lambda \operatorname{Id}_p + X^\top X)^{-1} X^\top \mathbb{E}(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top) X (\lambda \operatorname{Id}_p + X^\top X)^{-1} \\ &= \sum_{i=1}^{\mathrm{rg}(X)} \frac{s_i^2 \sigma^2}{(s_i^2 + \lambda)^2} \mathbf{v}_i \mathbf{v}_i^\top \end{aligned}$$

Rem one recovers $V^{\mathrm{OLS}} = \sum_{i=1}^{\mathrm{rg}(X)} \frac{\sigma^2}{s_i^2} \mathbf{v}_i \mathbf{v}_i^\top$ when $\lambda \to 0$

Rem one find a null variance when $\lambda \to \infty$

Exercise Show that the variance of when X is orthogonal is $\sigma^2 (1 + \lambda)^{-2} \operatorname{Id}_p$

Prediction risk

Homoscedastic assumption: $\mathbb{E}(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\top) = \sigma^2 \,\mathrm{Id}_n$

Quadratic prediction risk $\mathbb{E}\|X\boldsymbol{\theta}^\star - X\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}\|^2$ under the homoscedastic assumption:

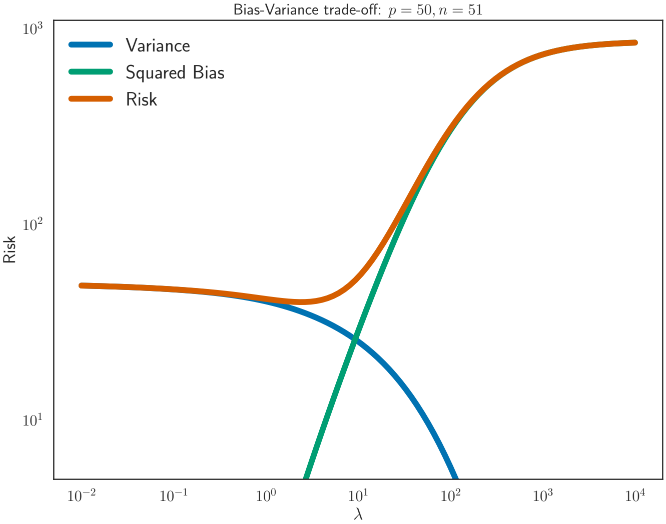
$$R_{\mathrm{pred}}(\boldsymbol{\theta}^\star, \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}) = \mathbb{E}\left[(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \boldsymbol{\theta}^\star)^\top (X^\top X)(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \boldsymbol{\theta}^\star)\right]$$

Explicit computation (begins as for OLS):

$$\begin{aligned}
R_{\mathrm{pred}}(\boldsymbol{\theta}^\star, \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}) &= \mathbb{E}\left[(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \boldsymbol{\theta}^\star)^\top (X^\top X)(\hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}} - \boldsymbol{\theta}^\star)\right] \\
&= \mathbb{E}\left[(X(X^\top X + \lambda \,\mathrm{Id}_p)^{-1} X^\top \boldsymbol{\varepsilon})^\top (X(X^\top X + \lambda \mathrm{Id}_p)^{-1} X^\top \boldsymbol{\varepsilon})\right] \\
&\quad + \lambda^2 \boldsymbol{\theta}^{\star\top} (X^\top X + \lambda \,\mathrm{Id}_p)^{-2} \boldsymbol{\theta}^\star \\
&= \sum_{i=1}^{\mathrm{rg}(X)} \frac{s_i^4 \sigma^2}{(s_i^2 + \lambda)^2} + n^2 \lambda^2 \boldsymbol{\theta}^{\star\top} (X^\top X + \lambda \,\mathrm{Id}_p)^{-2} \boldsymbol{\theta}^\star
\end{aligned}$$

Rem $\lim_{\lambda \to 0} R_{\mathrm{pred}}(\boldsymbol{\theta}^\star, \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}) = \mathrm{rg}(X)\sigma^2$, $\lim_{\lambda \to \infty} R_{\mathrm{pred}}(\boldsymbol{\theta}^\star, \hat{\boldsymbol{\theta}}_\lambda^{\mathrm{rdg}}) = \|X\boldsymbol{\theta}^\star\|_2^2$

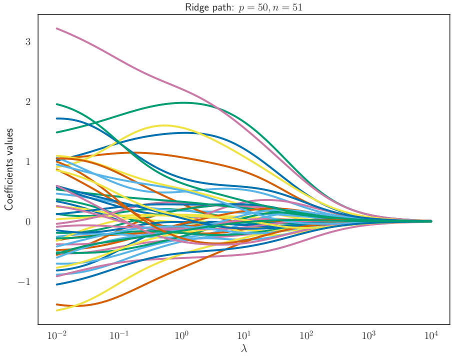
Bias / Variance: simulated example



$$\mathbf{X} \in \mathbb{R}^{51\times 50},\ \boldsymbol{\theta}^\star = (2, 2, 2, 2, 2, 0, \dots, 0)^\top$$

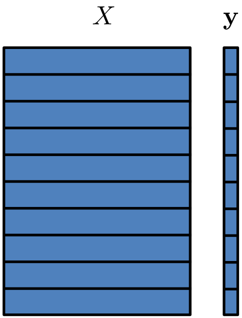
Choosing λ

```
n_features = 50; n_samples = 50
X = np.random.randn(n_samples, n_features)
theta_true = np.zeros([n_features, ])
theta_true[0:5] = 2.
y_true = np.dot(X, theta_true)
y = y_true + 1. * np.random.rand(n_samples,)
```



K-fold Cross-Validation ($K = 10$)

- Choose a grid of r λ's to test: $\lambda_1, \ldots, \lambda_r$
- Divide $(X, \mathbf{y})$ into K blocks (sample-wise):



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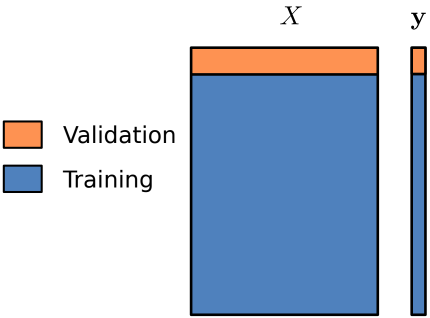

$k = 1$

1. Compute with the training part the estimators for $\lambda_1, \dots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \dots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
2. Evaluate the (prediction) error $\mathrm{Error}_1^k, \dots, \mathrm{Error}_r^k$ over the validation part,

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- Choose a grid of r λ's to test: $\lambda_1, \ldots, \lambda_r$
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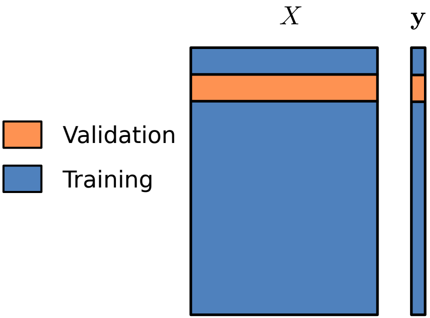

$k = 2$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
2. Evaluate the (prediction) error $\mathrm{Error}_1^k, \ldots, \mathrm{Error}_r^k$ over the validation part,

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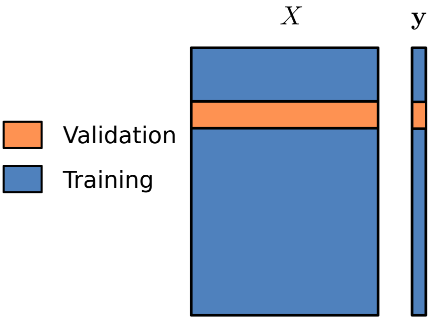

$k = 3$

1. Compute with the training part the estimators for $\lambda_1, \dots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \dots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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K-fold Cross-Validation ($K = 10$)

- Choose a grid of r λ's to test: $\lambda_1, \ldots, \lambda_r$
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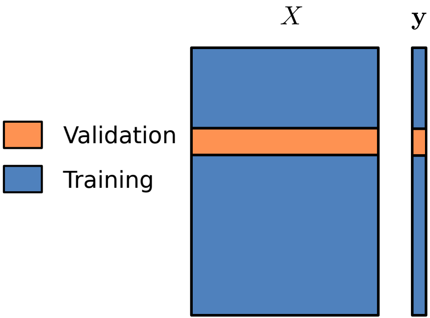

$k = 4$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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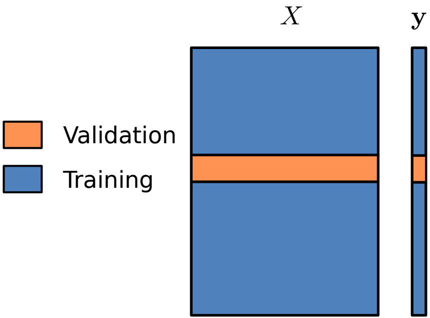
K-fold Cross-Validation ($K = 10$)

- Choose a grid of r λ's to test: $\lambda_1, \dots, \lambda_r$
- Divide $(X, \mathbf{y})$ into K blocks (sample-wise):



$k = 5$

1. Compute with the training part the estimators for $\lambda_1, \dots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \dots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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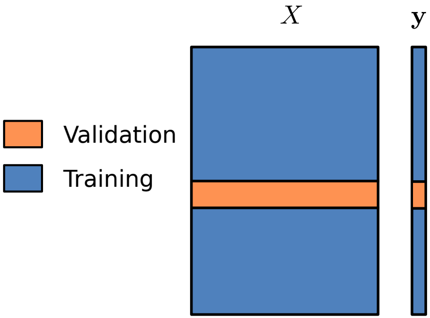
K-fold Cross-Validation ($K = 10$)

- Choose a grid of r λ's to test: $\lambda_1, \ldots, \lambda_r$
- Divide $(X, \mathbf{y})$ into K blocks (sample-wise):



$$k = 6$$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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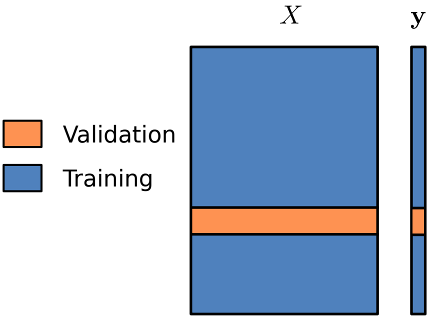

$k = 7$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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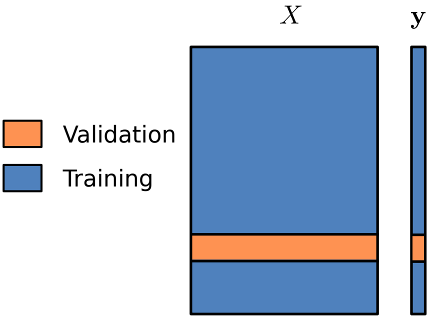

$k = 8$

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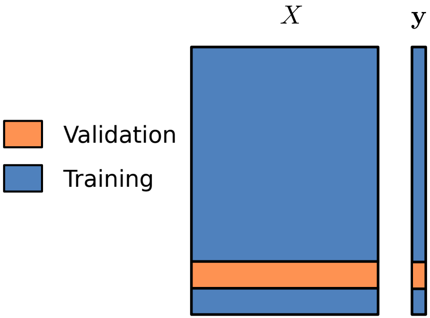

$k = 9$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
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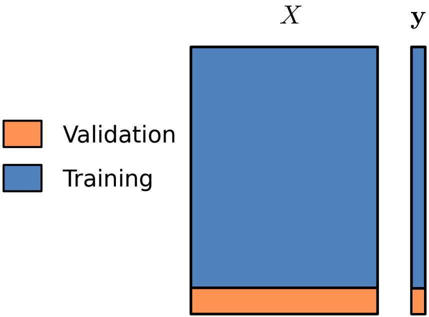

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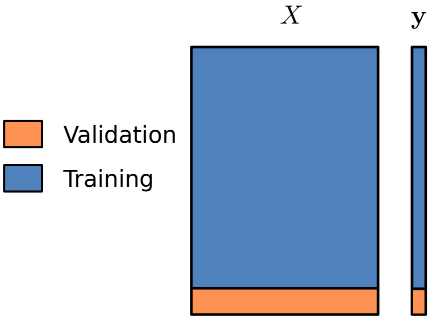


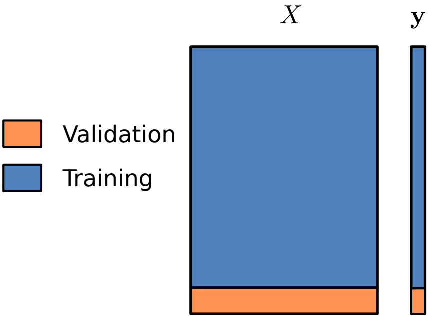
$k = 10$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
2. Evaluate the (prediction) error $\mathrm{Error}_1^k, \ldots, \mathrm{Error}_r^k$ over the validation part,

Parameter choice: averaging the previous errors over k gives $\widehat{\mathrm{Error}}_1, \ldots, \widehat{\mathrm{Error}}_r$. Then choose $i^* \in [\![1, r]\!]$ achieving the smallest one

K-fold Cross-Validation ($K = 10$)

- Choose a grid of r λ's to test: $\lambda_1, \ldots, \lambda_r$
- Divide $(X, \mathbf{y})$ into K blocks (sample-wise):



$$k = 10$$

1. Compute with the training part the estimators for $\lambda_1, \ldots, \lambda_r$: $\hat{\boldsymbol{\theta}}^{\lambda_1}, \ldots, \hat{\boldsymbol{\theta}}^{\lambda_r}$
2. Evaluate the (prediction) error $\mathrm{Error}_1^k, \ldots, \mathrm{Error}_r^k$ over the validation part,

<u>Parameter choice</u>: averaging the previous errors over k gives $\widehat{\mathrm{Error}}_1, \ldots, \widehat{\mathrm{Error}}_r$.
Then choose $i^* \in [\![1, r]\!]$ achieving the smallest one

<u>Re-calibration</u>: compute $\hat{\boldsymbol{\theta}}^{\lambda_{i^*}}$ over the whole sample

CV in practice

Extreme cases of CV

- $K = 1$ impossible, needs $K = 2$
- $K = n$, "*leave-one-out*" strategy (*cf.***Jackknife**): as many blocks as observations
  Rem $K = n$ (often) computationally efficient but unstable

Practical advice:

- "randomise the sample" : having samples in random order avoid artifacts block (each fold needs to be representative of the whole sample!)
- standard choices: $K = 5, 10$

Alternatives: random partition validation/test, time series variants, etc.

http://scikit-learn.org/stable/modules/cross_validation.html

CV variants `sklearn`

Crucial points: the structures train/test artificially created should represent faithfully the underlying learning problem

Classical alternatives:

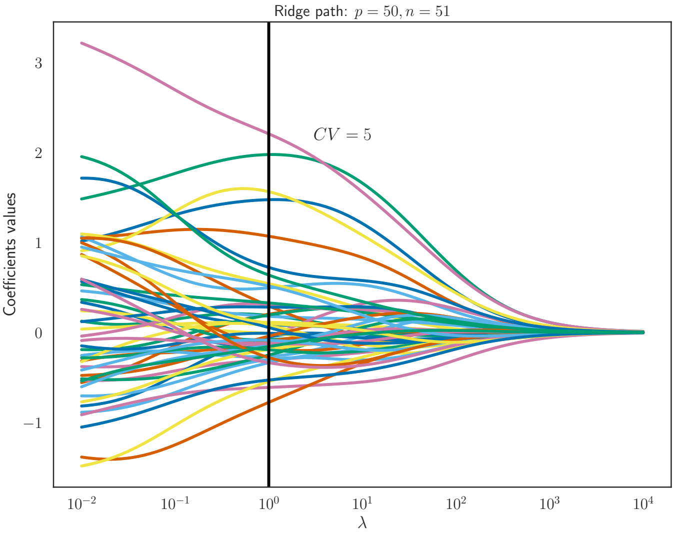
- random partitioning in train/test sets (*cf.*`train_test_split`)
- Time series variant: `TimeSeriesSplit` (never predict the past with future information)
- For classification tasks with unbalanced classes `StratifiedKFold`

Rem averaging estimators (with weights reflecting their performance) is also relevant for prediction

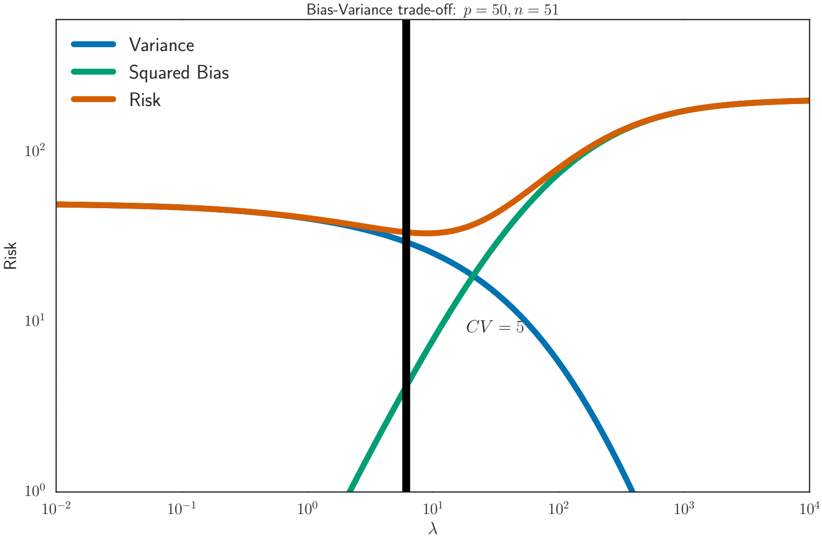
More details:

http://scikit-learn.org/stable/modules/cross_validation.html

Choosing λ : example with $CV = 5$ (I)



Choosing λ : example with $CV = 5$ (II)



Algorithms to compute the *Ridge* estimator

- `'svd'`: most stable method, useful for computing many λ's cause the SVD price is paid only once
- `'cholesky'` : matrix decomposition leading to a close form solution `scipy.linalg.solve`
- `'sparse_cg'`: conjugate gradient descent, useful also for sparse cases and high dimension (set `tol`/`max_iter` to a small value)
- stochastic gradient descent approaches : if n is huge

*cf.*the code of `Ridge`, `ridge_path`, `RidgeCV` in the module `linear_model` of `sklearn`

Rem it is rare to compute the *Ridge* estimator only for one single λ

Rem crucial issue of computing SVD for huge matrices...