

# Lecture 2: Linear Methods for Regression

Readings: ESL (Ch. 3), ISL (Ch. 3, 6), Bach (Ch. 3); code

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# Outline

- 1 Linear Regression and Least Squares
- 2 Challenges for OLS
- 3 Subset Selection Methods
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# Linear Regression Models

Goal: Given inputs/features  $X_1, \dots, X_p$  (each  $X_i \in \mathbb{R}$ ), predict an output  $Y \in \mathbb{R}$ .

## Definition 1: Linear Regression Model

The linear regression model has the form:

$$f(X) = \beta_0 + \sum_{j=1}^p X_j \beta_j = X^T \beta.$$

Here,  $X = (1, X_1, \dots, X_p) \in \mathbb{R}^{p+1}$  is the augmented input vector, and  $\beta = (\beta_0, \beta_1, \dots, \beta_p) \in \mathbb{R}^{p+1}$  is the vector of model parameters (unknown).

- ▶ The linear model either assumes the regression function  $\mathbb{E}[Y|X]$  is linear or that the linear model is a reasonable assumption.
- ▶ Note that  $f$  is linear in  $\beta$ . In general, it needs not be linear in  $X$ :  $f(X) = \varphi(X)^T \beta$  for some feature map  $\varphi : \mathbb{R}^{p+1} \rightarrow \mathbb{R}^{p+1}$ .
- ▶ The ERM problem can be solved easily using linear algebra.

# Ordinary Least Squares (OLS)

We fit the model by minimizing the **Residual Sum of Squares (RSS)**:

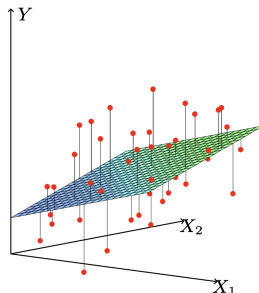
$$RSS(\beta) = \sum_{i=1}^N (y_i - f(x_i))^2 = (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) = \|\mathbf{y} - \mathbf{X}\beta\|_2^2;$$

or, equivalently, minimizing the empirical risk for squared-error loss:

$$\hat{R}_N(\beta) = \frac{1}{N} RSS(\beta) \text{ (also denoted } MSE(\beta)).$$

Denoting  $d := p + 1$ , here  $\mathbf{X}$  is the  $N \times d$  matrix (design matrix) with each row being an input row vector  $(1, \mathbf{x}_i^T)$ ,  $\mathbf{y}$  is the column vector of  $d$  outputs, and  $\beta$  is the  $d$ -vector of parameters. The entire set of predictions is:

$$\hat{\mathbf{y}} = \mathbf{X}\beta \in \mathbb{R}^N.$$



# Solution to the OLS

$$\hat{\beta} = \arg \min_{\beta} \sum_{i=1}^n (y_i - x_i^T \beta)^2 = \arg \min_{\beta} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta).$$

## Proposition 1: OLS Solution

Assuming that  $\mathbf{X}$  has full column rank so that  $\mathbf{X}^T \mathbf{X}$  is invertible (why?), the unique solution of the ERM problem is given by:

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$$

## Proof.

See blackboard.



- ▶ We call  $\hat{\beta}$  the OLS estimator.
- ▶ The predicted values at an input vector  $x_0$  is  $\hat{f}(x_0) = (1, x_0^T)^T \hat{\beta}$ .
- ▶ The fitted vector at the training inputs is  $\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} =: \mathbf{H}\mathbf{y}$ , where  $\hat{y}_i = \hat{f}(x_i)$ .

❗ How should we compute  $\hat{\beta}$  numerically when  $d$  is large?

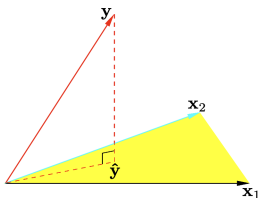
# Geometric Interpretation of OLS Estimator

The OLS solution has an elegant geometric interpretation based on projections.

- ▶ We define the **projection matrix** (or "hat" matrix) as:

$$\mathbf{\Pi} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$$

- ▶ So,  $\hat{\mathbf{y}} = \mathbf{\Pi} \mathbf{y}$ . This means  $\hat{\mathbf{y}}$  is the **orthogonal projection** of  $\mathbf{y}$  onto the column space of  $\mathbf{X}$  (show this).
- ▶ The residual vector  $\hat{\mathbf{e}} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{\Pi}) \mathbf{y}$  is the projection of  $\mathbf{y}$  onto the subspace orthogonal to the column space of  $\mathbf{X}$ .



❗ What if  $\mathbf{X}$  does not have full column rank?  $N \geq d$  vs.  $N < d$  case?

# Assumptions on True Data Distribution

To analyze the properties of our estimator  $\hat{\beta}$ , we assume a data-generating process:

$$y_i = \beta_0 + \sum_{j=1}^p x_{ij}\beta_j^* + \varepsilon_i \quad \text{for } i = 1, \dots, N,$$

for some  $\beta^* \in \mathbb{R}^d$ , where the errors  $\varepsilon_i$  are independent, and

- ▶  $\mathbb{E}[\varepsilon_i] = 0$
- ▶  $\text{Var}(\varepsilon_i) = \sigma^2$  for some constant  $\sigma > 0$  (homoscedasticity).

We focus on the **fixed design** setting, where we treat  $x_i$  as fixed (non-random). Our goal is to minimize  $R(\beta) = \frac{1}{N} \mathbb{E}_{\mathbf{y}} \|\mathbf{y} - \mathbf{X}\beta\|_2^2$ , where  $\mathbf{X}$  is deterministic.

💡 A more realistic setting is the **random design** setting, where both the inputs and outputs are assumed to be random and sampled i.i.d.. But the analysis of  $\hat{\beta}$  for this setting is more complicated (see Ch. 3.8 in Bach).

# Risk Decomposition for OLS Estimator

Let  $d := p + 1$  and denote by  $R^*$  the minimum value of  $R(\beta) := \mathbb{E}_{\mathbf{y}} \frac{1}{N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2$  over  $\mathbb{R}^d$ , we can show that it is attained at  $\beta^*$  and is equal to  $\sigma^2$ .

## Proposition 2: Risk Decomposition for OLS Estimator

Assume  $\mathbf{X}^T \mathbf{X}$  is invertible. Under the linear model and the fixed design assumptions made earlier, for any  $\beta \in \mathbb{R}^d$ , we have  $R^* = \sigma^2$  and

$$R(\beta) - R^* = \|\beta - \beta^*\|_{\hat{\Sigma}}^2,$$

where  $\hat{\Sigma} = \mathbf{X}^T \mathbf{X} / N$  and  $\|\beta\|_Q^2 := \beta^T Q \beta$  (Mahalanobis distance).

Moreover, if  $\hat{\beta}$  is a random variable, then

$$\mathbb{E}[R(\hat{\beta})] - R^* = \|\mathbb{E}[\hat{\beta}] - \beta^*\|_{\hat{\Sigma}}^2 + \mathbb{E}[\|\hat{\beta} - \mathbb{E}[\hat{\beta}]\|_{\hat{\Sigma}}^2].$$

Proof.

See blackboard.





# Statistical Properties of OLS Estimator

## Proposition 3: Statistical Properties of OLS Estimator

Under the same set of assumptions used in Prop. 2,

- ▶  $\mathbb{E}[\hat{\beta}] = \beta^*$  (unbiased).
- ▶  $\text{Var}(\hat{\beta}) = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2$ .

## Proof.

See blackboard. □

We can estimate the variance  $\sigma^2$  using  $\hat{\sigma}^2 = \frac{1}{N-d} \text{RSS}(\hat{\beta})$  (check:  $\mathbb{E}[\hat{\sigma}^2] = \sigma^2$ ).

💡 If we further assume that the errors are Gaussian, i.e.  $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$  for all  $i$ , then  $\hat{\beta}$  is also Gaussian (with the above mean and variance) and is independent of  $\hat{\sigma}^2$ . Moreover, we can form tests of hypothesis and confidence intervals for the parameters  $\beta_j$  (see Ch. 3.2.1 in ESL).

# Excess Risk of OLS Estimator

## Theorem 1: Excess Risk of OLS Estimator

Under the same set of assumptions used in Prop. 2, the excess risk of the OLS estimator is  $\mathbb{E}[R(\hat{\beta})] - R^* = \frac{\sigma^2 d}{N}$ .

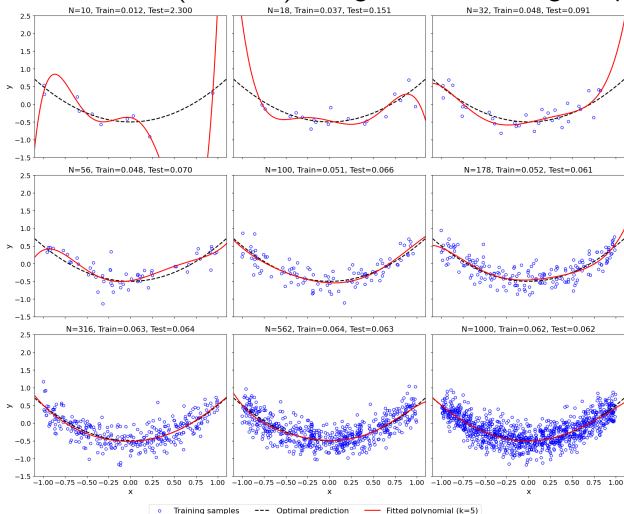
### Proof.

See blackboard. □

- ▶ For OLS regression, the training error underestimates (on average) the testing error by a factor of  $2\sigma^2 d/N$  (overfitting amount) – see Exercise 2.2.
- ▶ This result is for the fixed design setting. The random design setting is more involved mathematically (see Ch. 3.8 in Bach).
- ▶ The excess risk is large (compared to  $\sigma^2$ ) in high dimensions ( $d \geq N$ ).

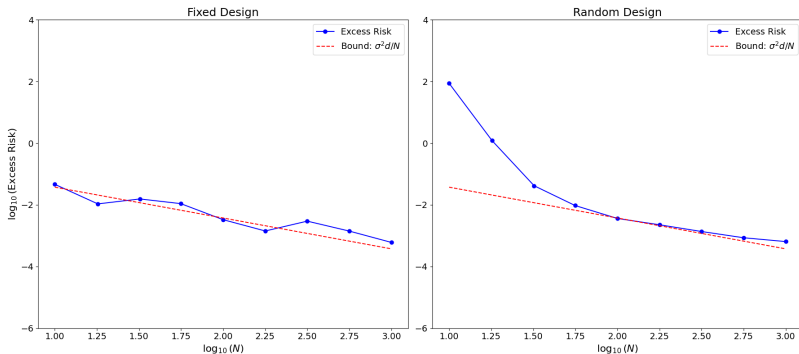
# Example: Polynomial Regression in 1D (Bach Ch. 3.5.2)

Same data generation setup as the one from Lecture 1. Look at regression with polynomials of order  $k = 5$  (so  $d = 6$ ), using different training sample size  $N$ .



# Expected Excess Risk vs. $N$

The expected excess risk is estimated using 32 replications of the experiment.



In-sample error vs. generalization error!

⚠ The bound seems to be valid only for large  $N$  in the random design setting.

# The Gauss-Markov Theorem

## Linear Unbiased Estimators

Consider any estimator  $\tilde{\beta}$  that is a linear function of  $\mathbf{y}$ , written as  $\tilde{\beta} = \mathbf{C}^T \mathbf{y}$ .

- ▶ For  $\tilde{\beta}$  to be an unbiased estimator of  $\beta$ ,  $\mathbf{C}$  must satisfy  $\mathbf{C}^T \mathbf{X} = \mathbf{I}$  (why?).
- ▶ The OLS estimator  $\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$  is one such estimator.

### Theorem 2: Gauss-Markov Theorem

The OLS estimator  $\hat{\beta}$  has the smallest variance among all linear unbiased estimators.

This means that for any other linear unbiased estimator  $\tilde{\beta}$ ,  $\text{Var}(\tilde{\beta}) - \text{Var}(\hat{\beta})$  is a positive semi-definite matrix.

### Proof.

See Exercise 2.1.



# When Does OLS Fail?

The variance of the coefficients is  $\text{Var}(\hat{\beta}) = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2$ . This can be large if:

- ▶ **Collinearity:** Predictors are highly correlated, making  $\mathbf{X}^T \mathbf{X}$  nearly singular (ill-conditioned). Small changes in the data can lead to huge swings in the coefficients.
- ▶ **High Dimensions ( $d > N$ ):** When the number of predictors exceeds the number of samples,  $\mathbf{X}^T \mathbf{X}$  is singular and the OLS solution is no longer unique (it admits a linear subspace of solutions).

Also, when  $d = N$ , the OLS leads to a perfect fit (typically not good for generalization to unseen data).

💡 The next families of methods—subset selection and shrinkage—are designed to address this problem by reducing model complexity and stabilizing the estimates.

# Subset Selection

The OLS model can be improved in two main ways by selecting a subset of predictors (retain a subset, discard the rest):

## Prediction Accuracy

- ▶ OLS can have high variance if  $d$  is large or predictors are collinear.
- ▶ Removing irrelevant predictors can reduce variance, potentially leading to a lower overall prediction error, even if it introduces a small amount of bias.

## Interpretation

- ▶ A smaller model with only the most important predictors is easier to understand and explain.
- ▶ It provides a parsimonious description of the process.

# Best-Subset and Stepwise Selection

## Best-Subset Selection

Finds, for each  $k \in \{0, 1, \dots, p\}$ , the subset of size  $k$  that gives the smallest RSS.

⚠ **Challenge:** Computationally infeasible for large  $p$ , as it requires checking  $2^p$  models.

## Stepwise Selection (Greedy Algorithms)

- ▶ **Forward-Stepwise:** Start with the null model. Iteratively add the one predictor that results in the largest decrease in RSS. A more constrained version is forward-stagewise regression.
- ▶ **Backward-Stepwise:** Start with the full model. Iteratively remove the one predictor that results in the smallest increase in RSS.

These are computationally efficient alternatives to best-subset selection but may not find the true best model.



# Shrinkage Methods (Regularization)

Instead of hard selection, shrinkage methods regularize the coefficients by shrinking them towards zero, which is a way of controlling model variance.

Examples are ridge regression, the Lasso, least angle regression (not covered).

## Definition 2: Ridge Regression

Ridge regression coefficients are the solution to the penalized ERM problem:

$$\hat{\beta}_{\lambda}^{\text{ridge}} = \arg \min_{\beta} \left\{ \frac{1}{N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_2^2 \right\}.$$

The term  $\lambda \|\beta\|_2^2$  is an L2 penalty and  $\lambda \geq 0$  is a complexity parameter.

See Exercise 2.3.

# Ridge Regression (L2 Regularization)

## Proposition 4: Ridge Least-Square Regression (RLS) Estimator

The solution has a closed form (stable even if  $\mathbf{X}^T \mathbf{X}$  is singular):

$$\hat{\beta}_{\lambda}^{\text{ridge}} = \frac{1}{N} \left( \frac{\mathbf{X}^T \mathbf{X}}{N} + \lambda \mathbf{I} \right)^{-1} \mathbf{X}^T \mathbf{y} =: \mathbf{H}_{\lambda} \mathbf{y},$$

where  $\mathbf{I}$  is the  $d \times d$  identity matrix.

## Proof.

See blackboard. □

- ▶ As  $\lambda \rightarrow \infty$ , the coefficients are shrunk to zero.
- ▶ Ridge is effective when many predictors have small-to-moderate effects. It does not set any coefficients to exactly zero (no variable selection).
- ▶ Simple relation between  $\hat{\beta}$  and  $\hat{\beta}_{\lambda}^{\text{ridge}}$  when the inputs are orthonormal (see Exercise 2.4).

# Excess Risk of Ridge Least-Square Estimator

## Proposition 5: Excess Risk of RLS Estimator

Under the same assumptions as the ones in Proposition 2-3 for the OLS estimator, the ridge least-square estimator has the following excess risk:

$$\mathbb{E}[R(\hat{\beta}_{\lambda}^{\text{ridge}})] - R^* = \underbrace{\lambda^2(\beta^*)^T(\hat{\Sigma} + \lambda I)^{-2}\hat{\Sigma}\beta^*}_{\text{bias}} + \underbrace{\frac{\sigma^2}{N}\text{tr}[\hat{\Sigma}^2(\hat{\Sigma} + \lambda I)^{-2}]}_{\text{variance}}.$$

**Proof.**

See Exercise 2.5. □

Based on the expression for the risk, we can tune  $\lambda$  to obtain a potentially better bound than with the OLS (e.g., Proposition 3.8 in Bach).

# The Lasso (L1 Regularization)

The Lasso can perform both shrinkage and automatic variable selection.

## Definition 3: The Lasso

The Lasso coefficients are the solution to:

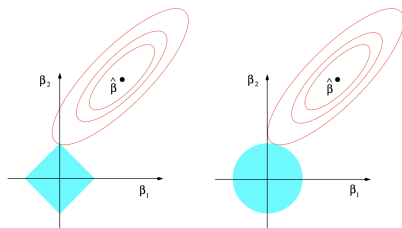
$$\hat{\beta}_{\lambda}^{\text{lasso}} = \arg \min_{\beta} \left\{ \frac{1}{N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_1 \right\}.$$

The term  $\lambda \|\beta\|_1$  is an L1 penalty and  $\lambda \geq 0$  is a complexity parameter.

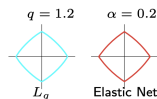
- ▶ The  $L_1$  penalty performs continuous shrinkage like Ridge.
- ▶ Crucially, due to the nature of the  $|\cdot|$  function, it is able to shrink some coefficients to be **exactly zero**. Thus, it performs automatic variable selection, yielding sparse models.
- ▶ There is no closed-form solution; it's solved via iterated methods such as coordinate descent.

# Geometric Interpretation: Ridge vs. Lasso

The difference between Ridge and Lasso can be viewed as optimizing RSS subject to different constraints. Let's look at  $p = 2$  case:



**FIGURE 3.11.** Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions  $|\beta_1| + |\beta_2| \leq t$  and  $\beta_1^2 + \beta_2^2 \leq t^2$ , respectively, while the red ellipses are the contours of the least squares error function.



**FIGURE 3.13.** Contours of constant value of  $\sum_j |\beta_j|^q$  for  $q = 1.2$  (left plot), and the elastic-net penalty  $\sum_j (\alpha \beta_j^2 + (1 - \alpha) |\beta_j|)$  for  $\alpha = 0.2$  (right plot). Although visually very similar, the elastic-net has sharp (non-differentiable) corners, while the  $q = 1.2$  penalty does not.

⚠ Obtaining excess risk bounds for the Lasso estimator is much more involved than the OLS and RLS estimator (see Ch. 8 in Bach).

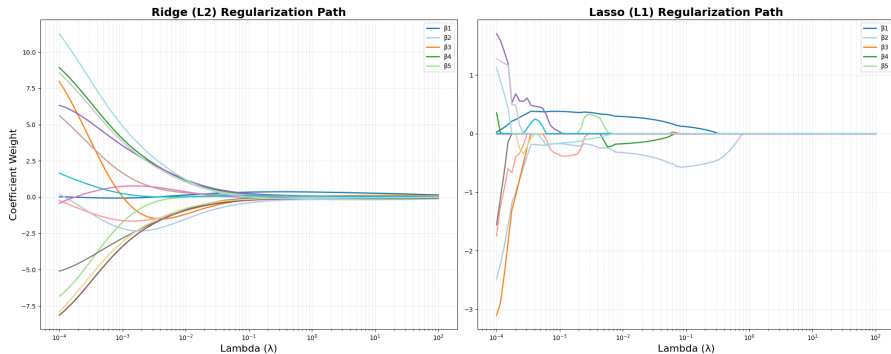
# Empirical Demonstration: OLS vs. RLS vs. Lasso

- ▶ Create synthetic data from  $f(x) = 1.5x^3 - 0.8x^2 + 0.3x + 0.1$  with added Gaussian noise.
- ▶ Generate 150 samples uniformly from  $[-1, 1]$ .
- ▶ Split into training (60%), validation (20%), and test (20%).

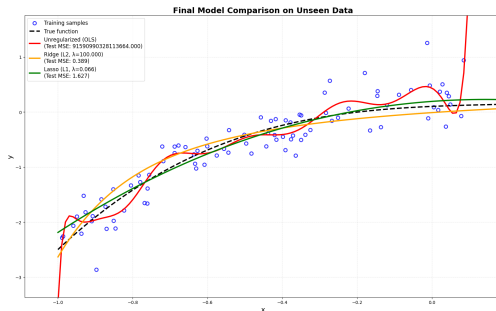
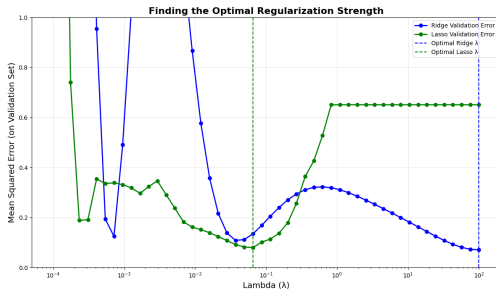
💡 Fit Ridge (L2) and Lasso (L1) regression models with degree-15 polynomial features (so  $d = 16$ ) on the training data. Vary  $\lambda$  over a grid and identify optimal  $\lambda$  for each method (using the validation set).

💡 Compare test MSE of the RLS model with optimal  $\lambda$  vs. the Lasso model with optimal  $\lambda$  vs. the OLS model on the test data.

# Empirical Demonstration: OLS vs. RLS vs. Lasso



# Empirical Demonstration: OLS vs. RLS vs. Lasso

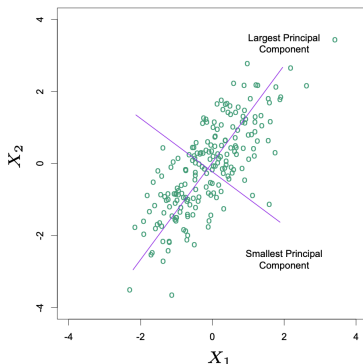




# Methods Using Derived Inputs

What if we have a large number of inputs, often very correlated?


One approach is to first derive a small number of linear combinations  $Z_m$ ,  $m = 1, \dots, M$ , of the original inputs  $X_j$ , and then use the  $Z_m$  in place of the  $X_j$  as inputs in the regression.



# Principal Components Regression (PCR)

The  $m$ th principal component of  $\mathbf{X}$  is the eigenvector associated with the  $m$ th largest eigenvalue of  $\mathbf{X}^T \mathbf{X}$ , assuming the columns of  $\mathbf{X}$  are centered.

- ▶ Compute the first  $M < p$  principal components  $Z_1, \dots, Z_M$  of the input matrix  $\mathbf{X}$ . These are linear combinations of the original predictors that capture the most variance.
- ▶ Regress the response  $\mathbf{y}$  on these  $M$  principal components using OLS.

 **Drawback:** The principal components are derived in an **unsupervised** manner. The directions of high variance in  $X$  might not be the directions that best predict  $Y$ . More on this later in the course.

# Partial Least Squares (PLS)

PLS is similar to PCR but addresses its main drawback by deriving the new input directions in a supervised way.

## Core Idea of PLS

PLS builds a sequence of derived inputs,  $Z_1, \dots, Z_M$ , by iteratively finding directions in the predictor space that are highly correlated with the response.

- ▶ At each step  $m$ , the direction is formed as a weighted average of the predictors, where the weights are the correlations of the predictors with the **current response vector**.
- ▶ After deriving a component  $Z_m$ , the predictors are made orthogonal to it. This ensures that the next component focuses on explaining the remaining variance in the data.

This supervised, iterative fitting process makes PLS a powerful tool for prediction and tends to perform well for datasets that have many correlated predictors and relatively few samples ( $p \gg N$ ).

# A High-Level Summary of Linear Methods

Method	Interpretability	Variable Selection	Common Use
OLS	High	No	Baseline, Inference ( $N > d$ )
Subset	Very High	Yes (Hard)	Small $d$ , Finding "true" model
Stepwise	High	Yes (Hard)	Larger $d$ , Efficient search
Ridge	Moderate	No	Prediction, Collinearity, $d > N$
Lasso	High	Yes (Soft)	Prediction with sparsity, $d > N$
PCR/PLS	Low	No	High-dim data, $d \gg N$

💡 Regularization provides a powerful framework to balance the bias-variance tradeoff.

💡 The Lasso has become quite popular because it offers a good compromise between the predictive power and stability of Ridge regression vs. the sparsity and interpretability of subset selection.

## Exercise 2

1. Prove the Gauss-Markov theorem (Theorem 2).
2. Under the same set of assumptions used in Proposition 2, show that the expected empirical risk (or expected training error) is equal to  $\mathbb{E}[\hat{R}(\hat{\beta})] = \frac{N-d}{N} \sigma^2$ . In particular, when  $N > d$ , deduce that an unbiased estimator of the noise variance  $\sigma^2$  is given by  $\frac{1}{N-d} \|\mathbf{y} - \mathbf{X}\hat{\beta}\|_2^2$ .
3. Show that the Ridge Regression solution  $\hat{\beta}_{\lambda}^{\text{ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$  is equivalent to solving the OLS problem subject to a spherical constraint, i.e., minimizing  $\|\mathbf{y} - \mathbf{X}\beta\|_2^2$  subject to  $\|\beta\|_2^2 \leq t$  for some  $t$ .
4. Show that in the case of orthonormal inputs, the RLS estimates are a scaled version of the OLS estimates:  $\hat{\beta}_{\lambda}^{\text{ridge}} = \hat{\beta} / (1 + \lambda)$ . The effective degrees of freedom of the ridge regression fit is defined as  $\text{df}(\lambda) = \text{tr}(\mathbf{X} \mathbf{H}_{\lambda})$ . Compute  $\text{df}(\lambda)$  and relate it to the scaling. What if the inputs are not orthonormal?
5. Prove Proposition 6. Validate the bias-variance decomposition empirically by providing a Python implementation to produce a figure like Figure 3.3 in Bach.