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Linear Regression Models

Segment 2 – Multiple Linear Regression Model

Topic 1 – Matrix Approach for Multiple Linear Regression Model

Sudarsan N.S. Acharya (sudarsan.acharya@manipal.edu)

Topics



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1. Matrix Notations for Data: Design Matrix
2. Dealing with Categorical Covariates
3. Multiple Linear Regression Models (MLRM) and assumptions
4. Ordinary Least Squares (OLS) Solution: Intuition, Geometry, & Algebraic Proof
5. Residual Vector and its Properties

Matrix Notations for Data: Design Matrix



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 $y^{(i)}$ = i th sample's **response** value, $x_j^{(i)}$ = i th sample's j th **predictor** value.

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$$\underbrace{\begin{bmatrix} r^{(1)} \\ r^{(2)} \\ \vdots \\ r^{(n)} \end{bmatrix}}_{\text{residual vector } \mathbf{r}} = \underbrace{\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}}_{\text{true response vector } \mathbf{y}} - \underbrace{\begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \dots & x_p^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \dots & x_p^{(2)} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} & \dots & x_p^{(n)} \end{bmatrix}}_{\text{design matrix } \mathbf{X}} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix}}_{\text{unknown coefficients vector } \boldsymbol{\beta}}$$

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$$\Rightarrow \mathbf{r} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}.$$

Dealing with Categorical Covariates



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	heatinghot air	heatinghot water/steam
electric	0	0
hot air	1	0
hot water/steam	0	1

Multiple Linear Regression Models (MLRM) and assumptions



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- The **random errors** for yet to be decided samples $i = 1, 2, \dots, n$ in the MLRM

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 3. the design matrix has full rank: $\text{rank}(\mathbf{X}) = p + 1$
 4. the random error vector is (multivariate) normally distributed: $\epsilon \sim N(0, \sigma^2 \mathbf{I})$.

Ordinary Least Squares (OLS) Solution: Intuition, Geometry, & Algebraic Proof



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- To find the coefficient estimates, just as in SLRM, we minimize the the sum of the squares of the residuals (**RSS**) for all samples in the dataset:

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$$\min \sum_{i=1}^n (r^{(i)})^2 = \sum_{i=1}^n \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \cdots + \beta_p x_p^{(i)} \right) \right)^2 .$$

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- Note that $\sum_{i=1}^n (r^{(i)})^2 = \underbrace{\left\| \begin{bmatrix} r^{(1)} \\ \vdots \\ r^{(n)} \end{bmatrix} \right\|}_{\text{norm of vector squared}}^2 = \|\mathbf{r}\|^2.$

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- The resulting solution is the OLS solution: $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$.

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- Using the equation $\mathbf{r} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}$, minimizing the **RSS** corresponds to minimizing $\|\mathbf{r}\|^2 = \text{minimizing } \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2.$
- The resulting solution is the OLS solution: $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$
- Full rank of the design matrix \mathbf{X} ensures the existence of $(\mathbf{X}^T \mathbf{X})^{-1}.$

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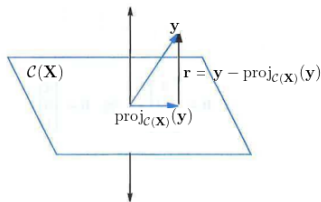
Ordinary Least Squares (OLS) Solution: Intuition, Geometry, & Algebraic Proof



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Minimizing $\|\mathbf{r}\|^2 = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 = \left\| \mathbf{y} - \underbrace{\left(\beta_0 \mathbf{x}_1 + \beta_1 \mathbf{x}_2 + \cdots + \beta_p \mathbf{x}_{p+1} \right)}_{\text{linear combination of columns of } \mathbf{X}} \right\|^2$ is

equivalent to solving the equation $\mathbf{X}\hat{\boldsymbol{\beta}} = \text{proj}_{\mathcal{C}(\mathbf{X})}(\mathbf{y})$ which represents the *orthogonal projection* of \mathbf{y} on to the column space of the design matrix $\mathcal{C}(\mathbf{X})$ (set of all possible linear combinations of the columns of \mathbf{X}):



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- Let $\text{proj}_{\mathcal{C}(\mathbf{X})}(\mathbf{y}) = \mathbf{X}\mathbf{z}$

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- Let $\text{proj}_{C(\mathbf{X})}(\mathbf{y}) = \mathbf{X}\mathbf{z} \Rightarrow \mathbf{r} = \mathbf{y} - \text{proj}_{C(\mathbf{X})}(\mathbf{y}) = \mathbf{y} - \mathbf{X}\mathbf{z}$.

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- Residual vector orthogonal to the column space of $\mathbf{X} \Rightarrow \mathbf{r} \perp \mathcal{C}(\mathbf{X})$

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 $\Rightarrow \mathbf{X}^T \mathbf{r} = \mathbf{0}$.

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- Using the fact that the design matrix \mathbf{X} has full rank (that is, its columns are linearly independent), we arrive at the unique OLS solution $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$.

Residual Vector and its Properties



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- This is a reiteration of the fact that linear regression works best on an average.