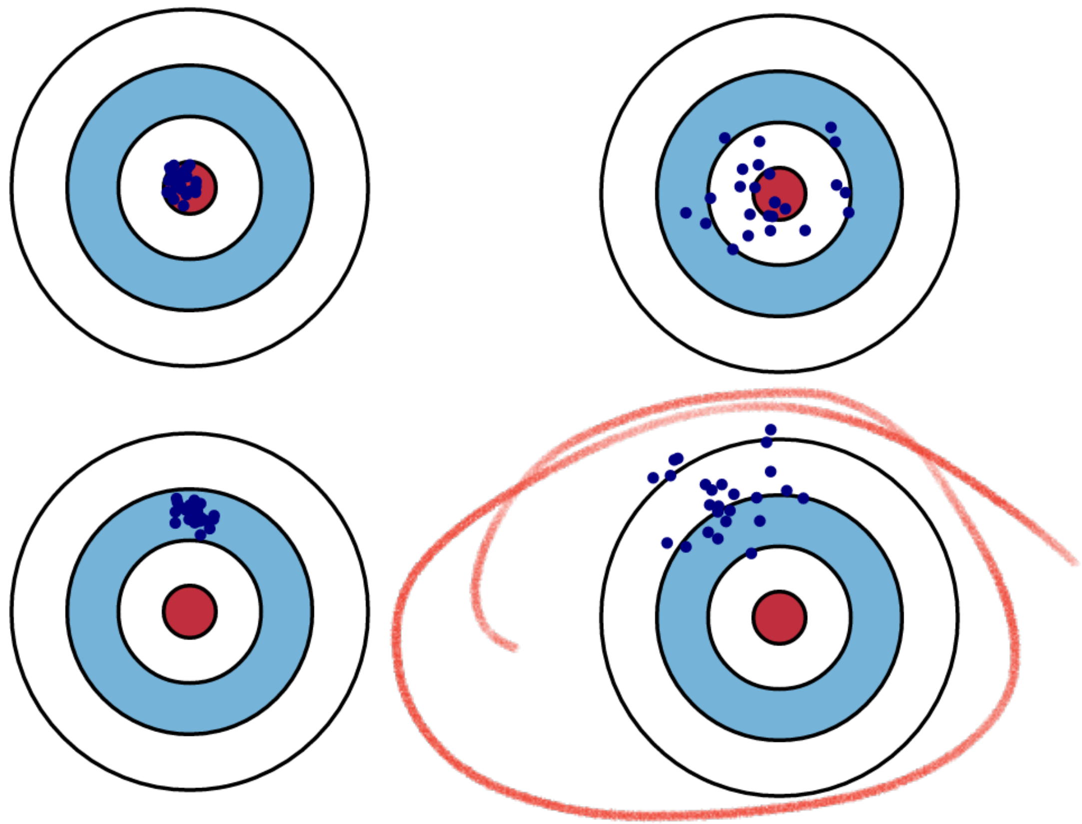
Bias-Variance Tradeoff
& Model Selection

Announcements

HW5 and P5 are coming out

Recap on Bias-Variance Tradeoff



Recap on Bias-Variance Tradeoff

Denote $h_{\mathscr{D}}$ as the ERM solution on dataset $\mathscr{D}$ w/ squared loss $\ell(h, x, y) = (h(x) - y)^2$

$\bar{h} = \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}]$

Recap on Bias-Variance Tradeoff

Denote $h_{\mathcal{D}}$ as the ERM solution on dataset $\mathcal{D}$ w/ squared loss $\ell(h, x, y) = (h(x) - y)^2$

What we have shown is the Bias-Variance decomposition:

$$\mathbb{E}_{\mathcal{D},x,y}(h_{\mathcal{D}}(x) - y)^2 = \underbrace{\mathbb{E}_{\mathcal{D},x}(h_{\mathcal{D}}(x) - \bar{h}(x))^2}_{\text{Variance}} + \underbrace{\mathbb{E}_x(\bar{h}(x) - \bar{y}(x))^2}_{\text{Bias}^2} + \mathbb{E}_{x,y}(\bar{y}(x) - y)^2$$

$\bar{y}$ = Bayes opt $= \mathbb{E}[y \mid x]$

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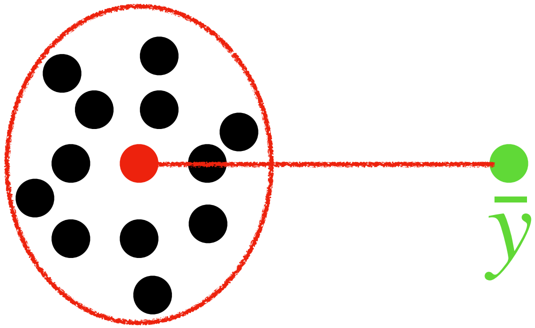
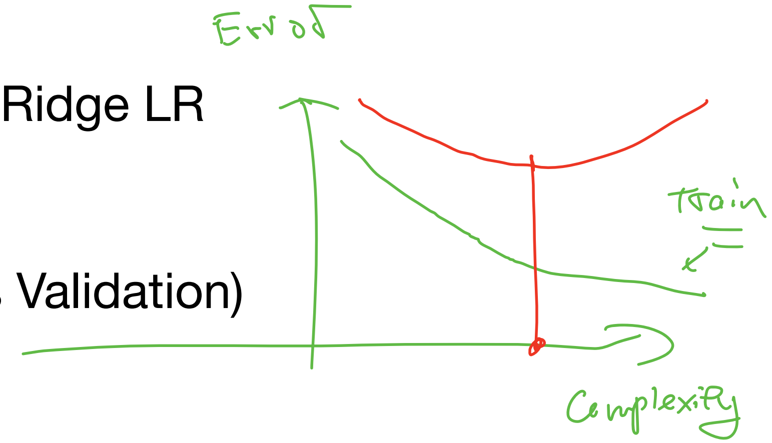


Outline of Today

1. Bias & Variance tradeoff demo on Ridge Linear Regression

2. Derivation of Bias / Variance for Ridge LR

2. Model selection in practice (Cross Validation)



Ridge Linear regression w/ fixed features and Gaussian noises

$x_i \in \mathbb{R}^d$

Let us consider the case where features are fixed, i.e., $x_1, \ldots, x_n$ fixed (no randomness)

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$$\text{But } y_i \sim (w^\star)^\top x_i + \epsilon_i,\ \epsilon_i \sim \mathcal{N}(0,1)$$

$$E[y|x] = (w^{*\top} x)$$

Ridge Linear regression w/ fixed features and Gaussian noises

Let us consider the case where features are fixed, i.e., $x_1, \ldots, x_n$ fixed (no randomness)

But $y_i \sim (w^\star)^\top x_i + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0,1)$

(This is called LR w/ fixed design)

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(This is called LR w/ fixed design)

$\epsilon_i \sim \mathcal{N}(0, 1)$

(So the only randomness of our dataset $\mathcal{D} = \{x_i, y_i\}$ is coming from the noises ϵ_i)

Ridge Linear regression

Ridge Linear Regression formulation

$$\hat{w} = \arg\min_{w} \sum_{i=1}^{n} (w^\top x_i - y_i)^2 + \lambda \|w\|_2^2$$

Regulazation

Ridge Linear regression

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What we will show now:

Larger λ (model becomes "simpler") => larger bias, but smaller variance

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$+\infty$

$\hat{w} - w^*$

$\mathrm{Var}(\hat{w})$

What we will show now:

Larger λ (model becomes “simpler”) => larger bias, but smaller variance

(Q: think about the case where $\lambda \to^{+} \infty$, what happens to $\hat{w}$?)

$\hat{w} = 0$

Ridge Linear regression

Demonstration for 2d ridge linear regression

$x_i \in R^2$

1. We create 5000 datasets: $\mathscr{D}_1, \mathscr{D}_2, \ldots, \mathscr{D}_{5000}$,

2. For a given λ, solve Ridge LR for each dataset, get $\hat{w}_1, \ldots, \hat{w}_{5000}$

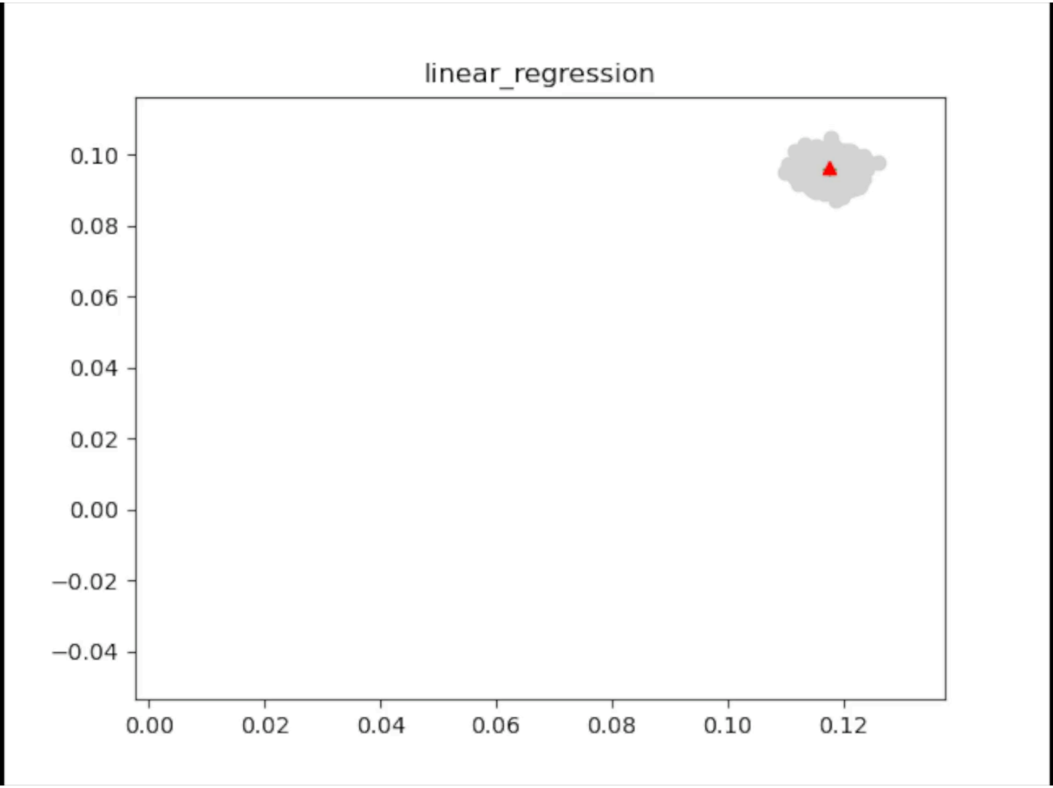
$\hat{w}_i \in R^2$

3. Estimate the mean $\bar{w} = \sum_i \hat{w}_i / 5000$

4. Plot $\hat{w}_1, \ldots, \hat{w}_{5000}$, and mean $\bar{w}$, and the optimal $w^\star$

Ridge Linear regression

We start with $\lambda = 0$, and gradually increase λ to $+\infty$:



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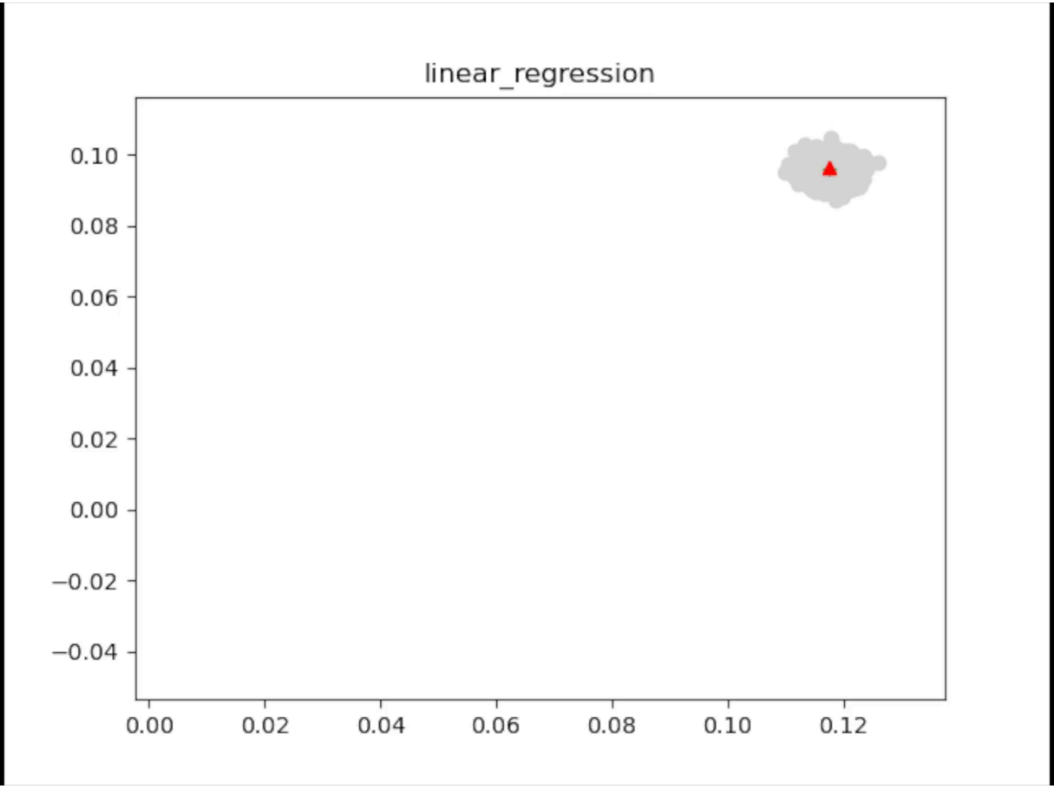

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Derivation of Bias and Variance for Ridge Linear regression

Denote $X = [x_1, \ldots, x_n] \in \mathbb{R}^{d \times n}, Y = [y_1, \ldots, y_n]^\top \in \mathbb{R}^n, \epsilon = [\epsilon_1, \ldots, \epsilon_n]^\top \in \mathbb{R}^n$

$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix}$$

Ridge LR in matrix / vector form:

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$\epsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

$$y_i = w^{*\top} x_i + \varepsilon_i$$

Derivation of Bias and Variance for Ridge Linear regression

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$$\hat{w} = \arg\min_{w} \|X^\top w - Y\|_2^2 + \lambda \|w\|_2^2$$

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Ridge LR in matrix / vector form:

$$\hat{w} = \arg\min_{w} \|X^\top w - Y\|_2^2 + \lambda \|w\|_2^2$$

Since $y_i = (w^\star)^\top x_i + \epsilon_i$ we have $Y = X^\top w^\star + \epsilon$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} - & x_1^\top & - \\ & \vdots & \\ - & x_n^\top & - \end{bmatrix} w^\star + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

The Expectation of the Ridge LR solution

Recall we have closed form solution for Ridge LR

$$\hat{w} = (XX^\top + \lambda I)^{-1} XY \; = (XX^\top + \lambda I)^{-1} X(X^\top w^\star + \epsilon)$$

$$Y = X^\top w^\star + \epsilon$$

$$\hat{w} - w^\star$$

$$\bar{w} = \mathbb{E}[\hat{w}]$$

$$\bar{w} - \hat{w}$$

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Source of the randomness of $\hat{w}$

$E[\hat{w}]$

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$$\mathbb{E}_\epsilon[\hat{w}] = (XX^\top + \lambda I)^{-1} X[X^\top w^\star + \mathbb{E}_\epsilon[\epsilon]]$$

$= 0$

$\mathbb{E}_\epsilon[\epsilon] = 0$

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$$= (XX^\top + \lambda I)^{-1} XX^\top w^\star$$

$= \bar{w}$

$\bar{w} - w^\star$

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$$= (XX^\top + \lambda I)^{-1} XX^\top w^\star$$

$$XX^\top = (XX^\top + \lambda I - \lambda I)$$

$$= (XX^\top + \lambda I)^{-1} (XX^\top + \lambda I - \lambda I) w^\star$$

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$$\bar{w} = \mathbb{E}_\epsilon[\hat{w}] = (XX^\top + \lambda I)^{-1}X[X^\top w^\star + \mathbb{E}_\epsilon[\epsilon]]$$

$$= (XX^\top + \lambda I)^{-1}XX^\top w^\star$$

$$= (XX^\top + \lambda I)^{-1}(XX^\top + \lambda I - \lambda I)w^\star = w^\star - \lambda(XX^\top + \lambda I)^{-1}w^\star$$

$$\bar{w} - w^\star = -\lambda(XX^\top + \lambda I)^{-1}w^\star$$

The Bias of Ridge Linear regression

$$\bar{w} = \mathbb{E}[\hat{w}] = w^\star - \lambda(XX^\top + \lambda)^{-1} w^\star$$

$\bar{w} - w^\star = -\lambda (XX^\top + \lambda)^{-1} w^\star$

Bias term: $\sum_{i=1}^{n} \left((\bar{w} - w^\star)^\top x_i \right)^2$

$\left(\bar{w}^\top x_i - w^{\star\top} x_i \right)^2$

The Bias of Ridge Linear regression

$$\bar{w} = \mathbb{E}[\hat{w}] = w^\star - \lambda(XX^\top + \lambda)^{-1} w^\star$$

$XX^T = \sum_{i=1}^{n} x_i x_i^T$

Bias term: $\sum_{i=1}^{n} \left((\bar{w} - w^\star)^\top x_i\right)^2$

$(a^T b)^2 = (a^T b \cdot b^T a)$

$$= \sum_{i=1}^{n} \left((\lambda(XX^\top + \lambda I)^{-1} w^\star)^\top x_i\right)^2$$

$\Rightarrow \sum_{i=1}^{n} (\lambda(XX^T + \lambda I)^{-1} w^*)^T x_i x_i^T (\lambda(XX^T + \lambda I)^{-1} w^*)$

$\Rightarrow (\lambda(XX^T + \lambda I)^{-1} w^*)^T XX^T (\lambda(XX^T + \lambda I)^{-1} w^*)$

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$$= \sum_{i=1}^{n} \left((\lambda(XX^\top + \lambda)^{-1} w^\star)^\top x_i \right)^2$$

$$= \lambda^2 (w^\star)^\top (XX^\top + \lambda I)^{-1} XX^\top (XX^\top + \lambda I)^{-1} w^\star$$

The Bias of Ridge Linear regression

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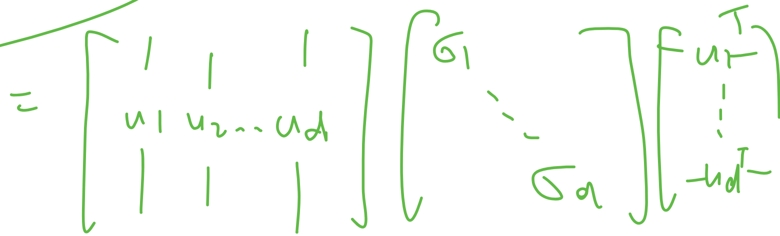
Eigendecomposition on $XX^\top = U\Sigma U^\top$



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Eigendecomposition on $XX^\top = U\Sigma U^\top$

$$= (w^\star)^\top U \begin{bmatrix} \frac{\sigma_1}{(\sigma_1/\lambda + 1)^2} & 0 & 0\ldots \\ 0 & \frac{\sigma_2}{(\sigma_2/\lambda + 1)^2} & 0\ldots \\ \ldots & \ldots & \ldots \\ 0, & \ldots & \frac{\sigma_d}{(\sigma_d/\lambda + 1)^2} \end{bmatrix} U^\top w^\star$$

The Bias of Ridge Linear regression

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Eigendecomposition on $XX^\top = U\Sigma U^\top$

$\lambda \to +\infty \quad \frac{\sigma_1}{(\sigma_1/\lambda+1)^2} \to \sigma_1$

$$= (w^\star)^\top U \begin{bmatrix} \frac{\sigma_1}{(\sigma_1/\lambda+1)^2} & 0 & 0\ldots \\ 0 & \frac{\sigma_2}{(\sigma_2/\lambda+1)^2} & 0\ldots \\ \cdots & \cdots & \cdots \\ 0, & \cdots & \frac{\sigma_d}{(\sigma_d/\lambda+1)^2} \end{bmatrix} U^\top w^\star$$

$w^{\star\top} X - w^\top X \hookrightarrow 0$

$\Rightarrow w^{\star\top} X$

Q: how does bias behave when $\lambda \to +\infty$

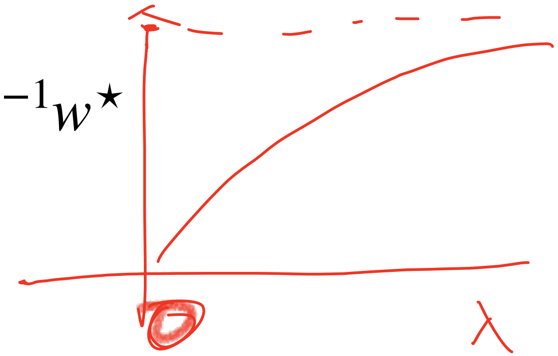
$\Rightarrow w^{\star\top} U \Sigma U^\top w^\star$

$= w^{\star\top} X X^\top w^\star$

$= \sum_{i=1}^{n} (w^{\star\top} x_i)^2$

The Bias of Ridge Linear regression

$$\text{Bias } = \lambda^2 (w^\star)^\top (XX^\top + \lambda I)^{-1} XX^\top (XX^\top + \lambda I)^{-1} w^\star$$



Eigendecomposition on $XX^\top = U\Sigma U^\top$

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Q: how does bias behave when $\lambda \rightarrow +\infty$

Q: how does bias behave when $\lambda \rightarrow 0$

The Variance of Ridge Linear regression

$$\bar{w} = \mathbb{E}[\hat{w}] = (XX^\top + \lambda I)^{-1} XX^\top w^\star$$

The Variance of Ridge Linear regression

closed-form expression

$$\bar{w} = \mathbb{E}[\hat{w}] = (XX^\top + \lambda I)^{-1} XX^\top w^\star$$

Variance term: $\sum_{i=1}^{n} \mathbb{E}(\hat{w}^\top x_i - \bar{w}^\top x_i)^2$

Random Expectation

The Variance of Ridge Linear regression

$$\bar{w} = \mathbb{E}[\hat{w}] = (XX^\top + \lambda I)^{-1} XX^\top w^\star$$

Variance term: $\sum_{i=1}^{n} \mathbb{E}(\hat{w}^\top x_i - \bar{w}^\top x_i)^2$

σ eigenvalues of $XX^\top$

$$= \sum_{i=1}^{d} \sigma_i^2 / (\sigma_i + \lambda)^2$$

The Variance of Ridge Linear regression

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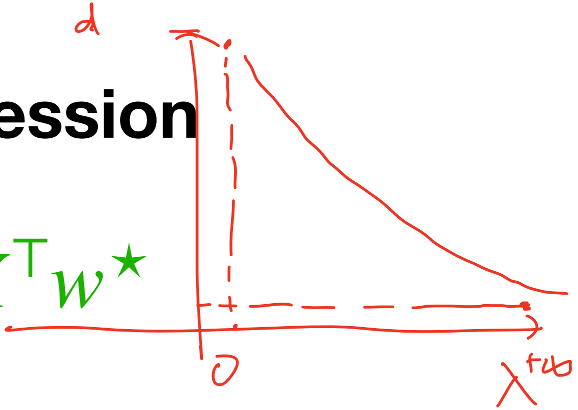
(Optional — tedious but basic computation, see note)

The Variance of Ridge Linear regression



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$$= \sum_{i=1}^{d} \sigma_i^2 / (\sigma_i + \lambda)^2$$

(Optional — tedious but basic computation, see note)

$\lambda = +\infty$: $\frac{\sigma^2}{(\sigma+\lambda)^2} = 0$

$\lambda = 0$

$\Rightarrow \frac{\sigma^2}{(\sigma+\lambda)^2} = 1$

$\sum_{i=1}^{d} \left(\frac{\sigma_i^2}{(\sigma_i+\lambda)^2}\right) = d$

Q: how does Var behave when $\lambda \to +\infty$

Q: how does Var behave when $\lambda \to 0$

Ridge Linear regression

Tuning λ allows us to control the generalization error of Ridge LR solution:

$$\mathbb{E}(\hat{w}^\top x - y)^2 = \text{Variance} + \text{Bias}^2 + \text{Inherent noise}$$

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The λ that minimizes Var + Bias^2

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How to select the best model from data

Examples:

1. Select the right order of polynomials for regression

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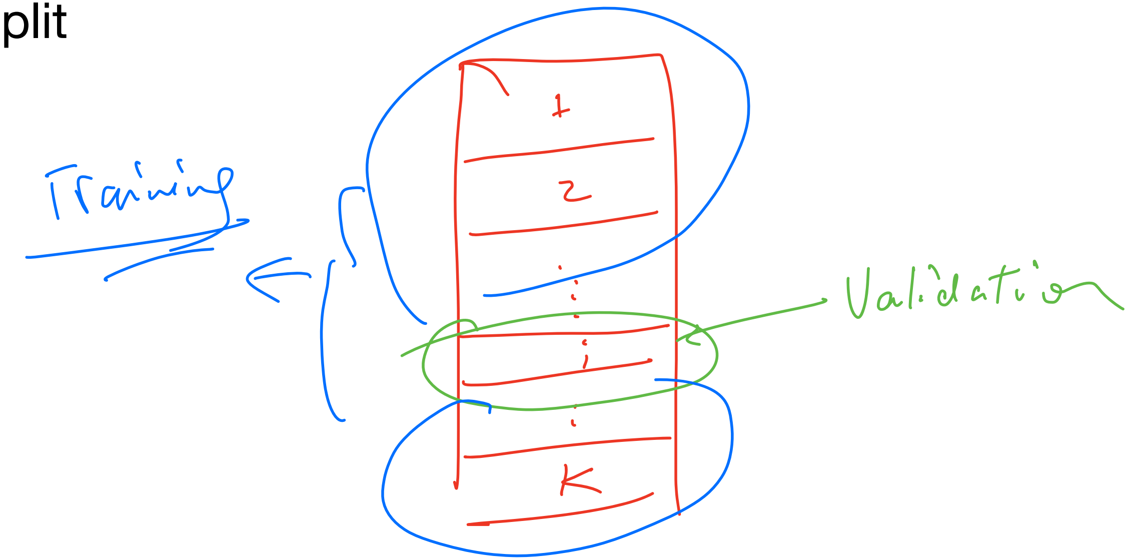
Select the right λ for Ridge LR

K-cross Validation

Cross Validation:

Random shuffle data, split the data into K folds

For i = 1 to K:



Select the right λ for Ridge LR

Cross Validation:

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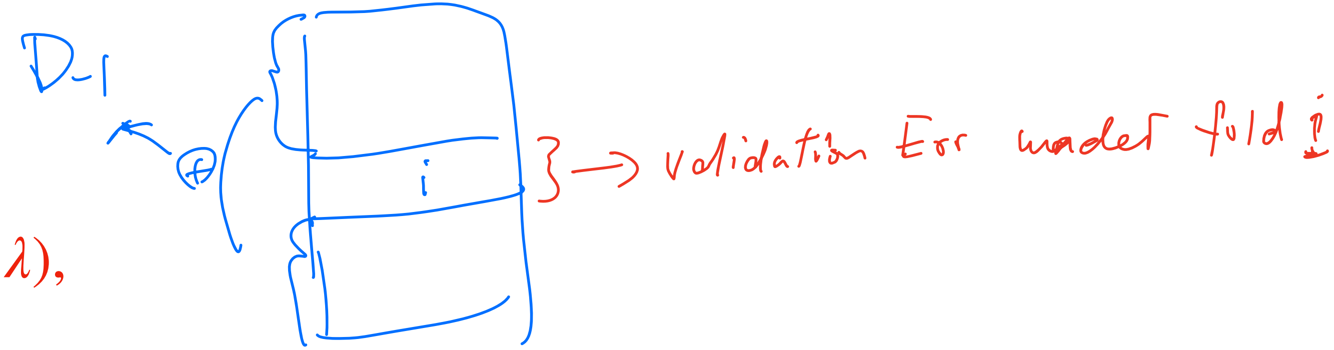
For i = 1 to K:

$\hat{w}_i$ = Ridge LR$(\mathscr{D}_{-i}, \lambda)$,



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For i = 1 to K:

$$\hat{w}_i = \text{Ridge LR}(\mathcal{D}_{-i}, \lambda),$$

$$\epsilon_{vad;i} = \sum_{x,y \in \mathcal{D}_i} (\hat{w}_i^\top x - y)^2 / |\mathcal{D}_i|$$

Select the right λ for Ridge LR

Cross Validation:

Random shuffle data, split the data into K folds

$|D| = $ # of points in D

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Output avg val-err over K folds: $\bar{\epsilon}_\lambda = \sum_{i=1}^{K} \epsilon_{vad;i} / K$

Select the right λ for Ridge LR

Cross Validation:

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$\approx \mathbb{E}_{x,y\sim P}(\hat{w}_i^\top x - y)^2$, i.e., test error of $\hat{w}_i$

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$\approx \mathbb{E}_{\mathscr{D}}\left[\mathbb{E}_{x,y\sim P}(\hat{w}_{\mathscr{D}}^\top x - y)^2\right]$, i.e.,

Generalization error of Ridge LR w/ λ

Select the right λ for Ridge LR

By numerating a set of possible $\lambda \in \mathbb{R}^+$, we select the one that has the smallest Cross-Valid error:

Select the right λ for Ridge LR

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For λ in [1e-5, 1e-4, … 1e4,1e5]:

Select the right λ for Ridge LR

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Split the data into K folds

For i = 1 to K:

$\hat{w}_i = \text{Ridge LR}(\mathscr{D}_{-i}, \lambda),$

$\epsilon_{vad;i} = \sum_{x,y \in \mathscr{D}_i} (\hat{w}_i^\top x - y)^2 / \ \mathscr{D}_i$

Output avg val-err over K folds: $\bar{\epsilon}_\lambda = \sum_{i=1}^{K} \epsilon_{vad;i} / K$

Generation Error of Ridge LR w/ λ

Select the right λ for Ridge LR

By numerating a set of possible $\lambda \in \mathbb{R}^+$, we select the one that has the smallest Cross-Valid error:

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Split the data into K folds

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$\hat{w}_i = \text{Ridge LR}(\mathcal{D}_{-i}, \lambda),$

$\epsilon_{vad;i} = \sum_{x,y \in \mathcal{D}_i} (\hat{w}_i^\top x - y)^2 / \ \mathcal{D}_i$

Output avg val-err over K folds: $\bar{\epsilon}_\lambda = \sum_{i=1}^{K} \epsilon_{vad;i} / K$

Select $\lambda^\star = \arg\min_\lambda \bar{\epsilon}_\lambda$

Select the right λ for Ridge LR

By numerating a set of possible $\lambda \in \mathbb{R}^+$, we select the one that has the smallest Cross-Valid error:

For λ in [1e-5, 1e-4, … 1e4,1e5]:

Split the data into K folds

For i = 1 to K:

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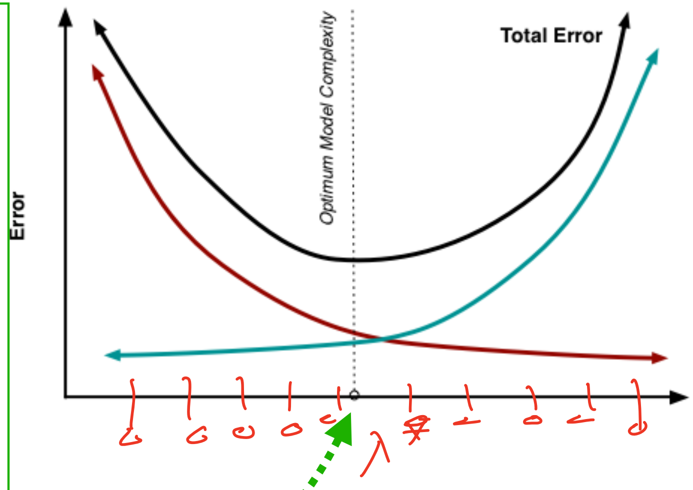

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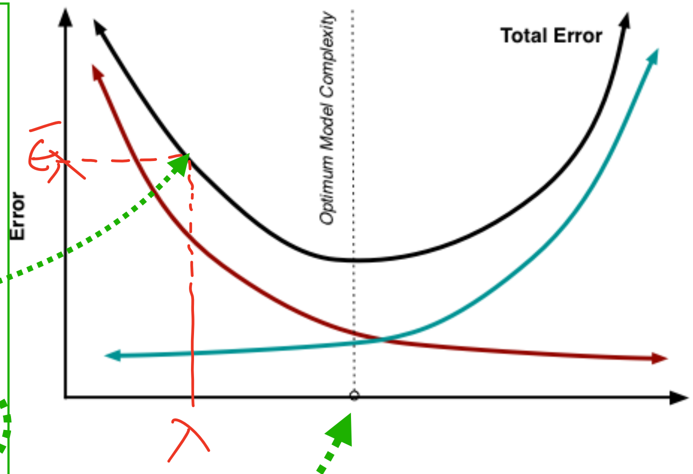
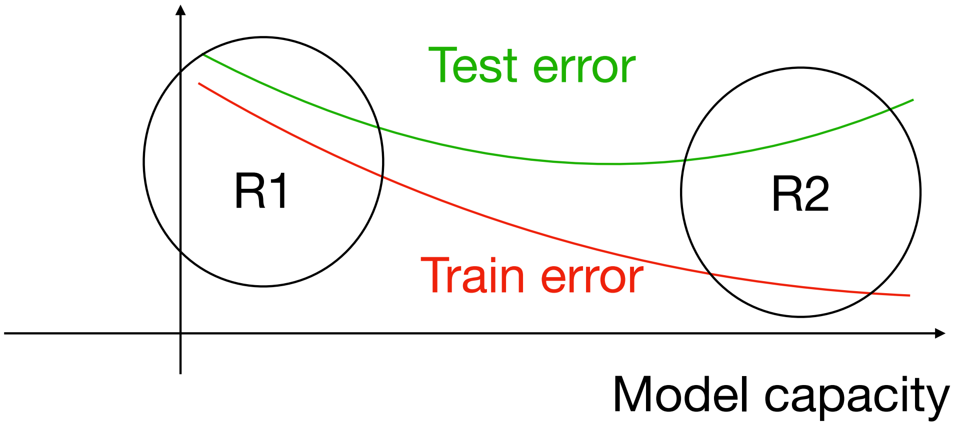
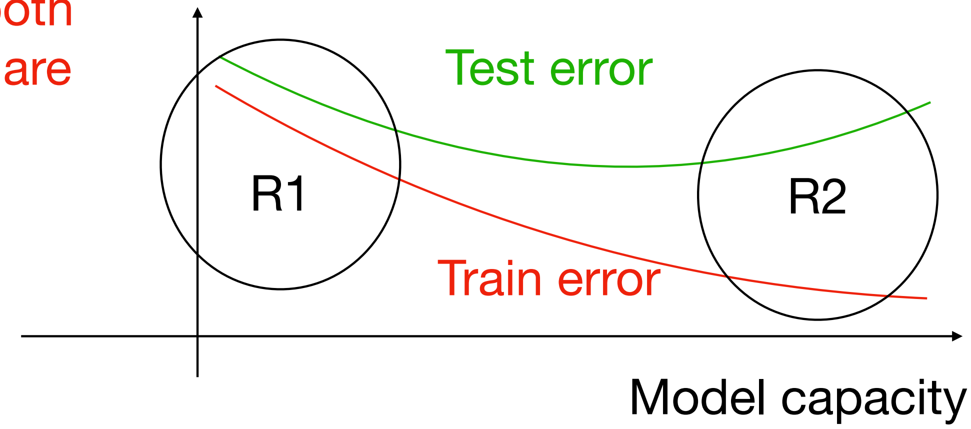


Practical Suggestions for combating over/under fitting



Practical Suggestions for combating over/under fitting

R1: Underfitting (both train and test errs are large)

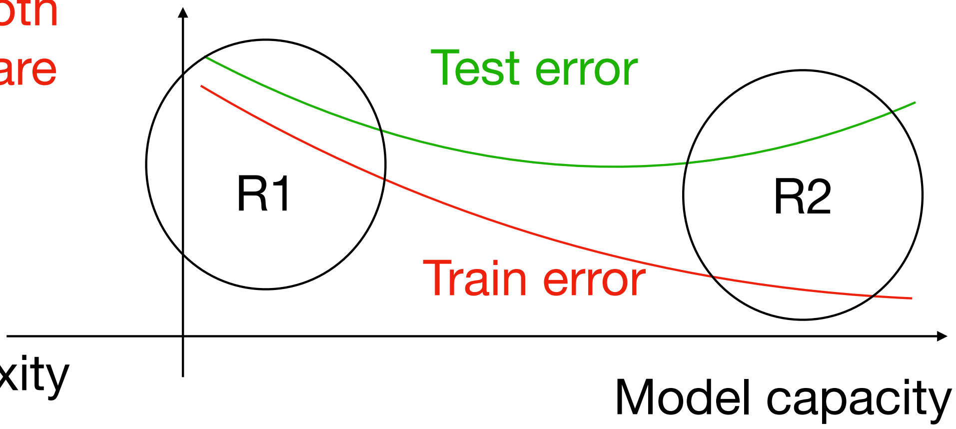


Practical Suggestions for combating over/under fitting

R1: Underfitting (both train and test errs are large)

Suggestions:

1. Increase complexity of models

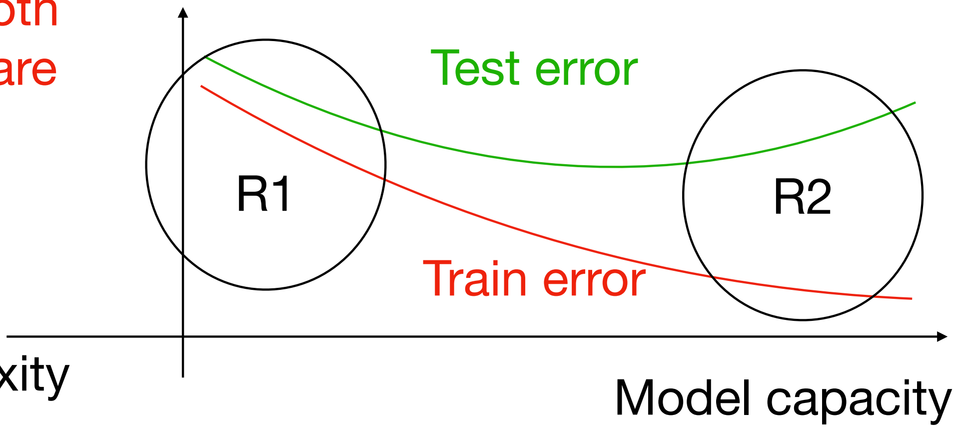


Practical Suggestions for combating over/under fitting

R1: Underfitting (both train and test errs are large)

Suggestions:

1. Increase complexity of models
2. More features



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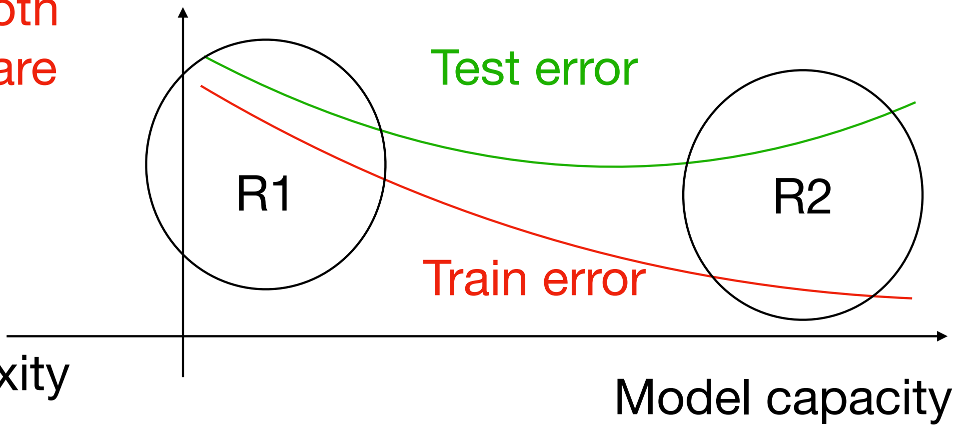

Suggestions:

1. Increase complexity of models

2. More features

3. Using Boosting (we will see it later)

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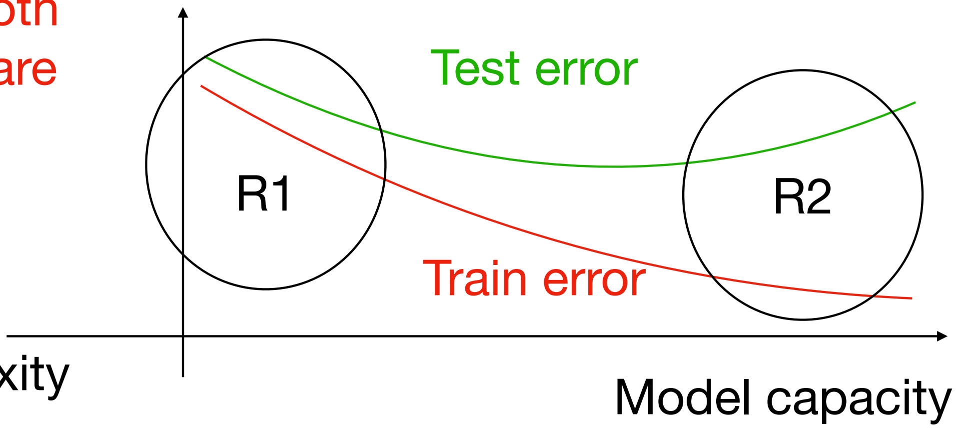

R2: overfitting (small train err but large test err)

Practical Suggestions for combating over/under fitting

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Suggestions:

1. Increase complexity of models

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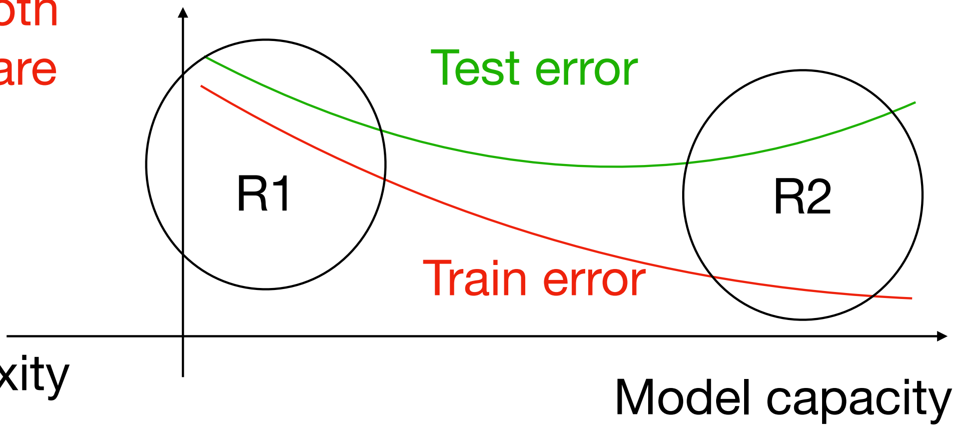


R2: overfitting (small train err but large test err)

Suggestions:

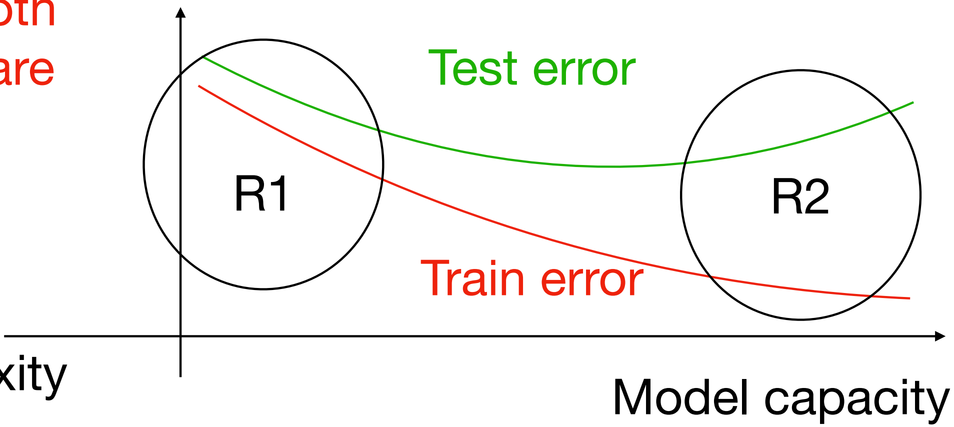
1. More train data

Practical Suggestions for combating over/under fitting

R1: Underfitting (both train and test errs are large)

Suggestions:

1. Increase complexity of models
2. More features
3. Using Boosting (we will see it later)



R2: overfitting (small train err but large test err)

Suggestions:

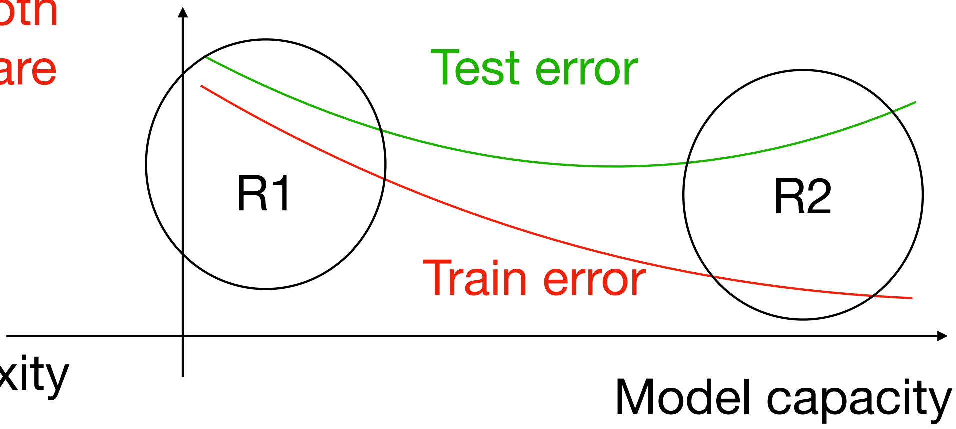
1. More train data
2. Reduce model capacity

Practical Suggestions for combating over/under fitting

R1: Underfitting (both train and test errs are large)

Suggestions:

1. Increase complexity of models
2. More features
3. Using Boosting (we will see it later)



R2: overfitting (small train err but large test err)

Suggestions:

1. More train data
2. Reduce model capacity
3. Using Bagging (we will see it later)