

Bias-Variance Tradeoff & Model Selection

Announcements

HW5 and P5 are coming out

Recap on Bias-Variance Tradeoff

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

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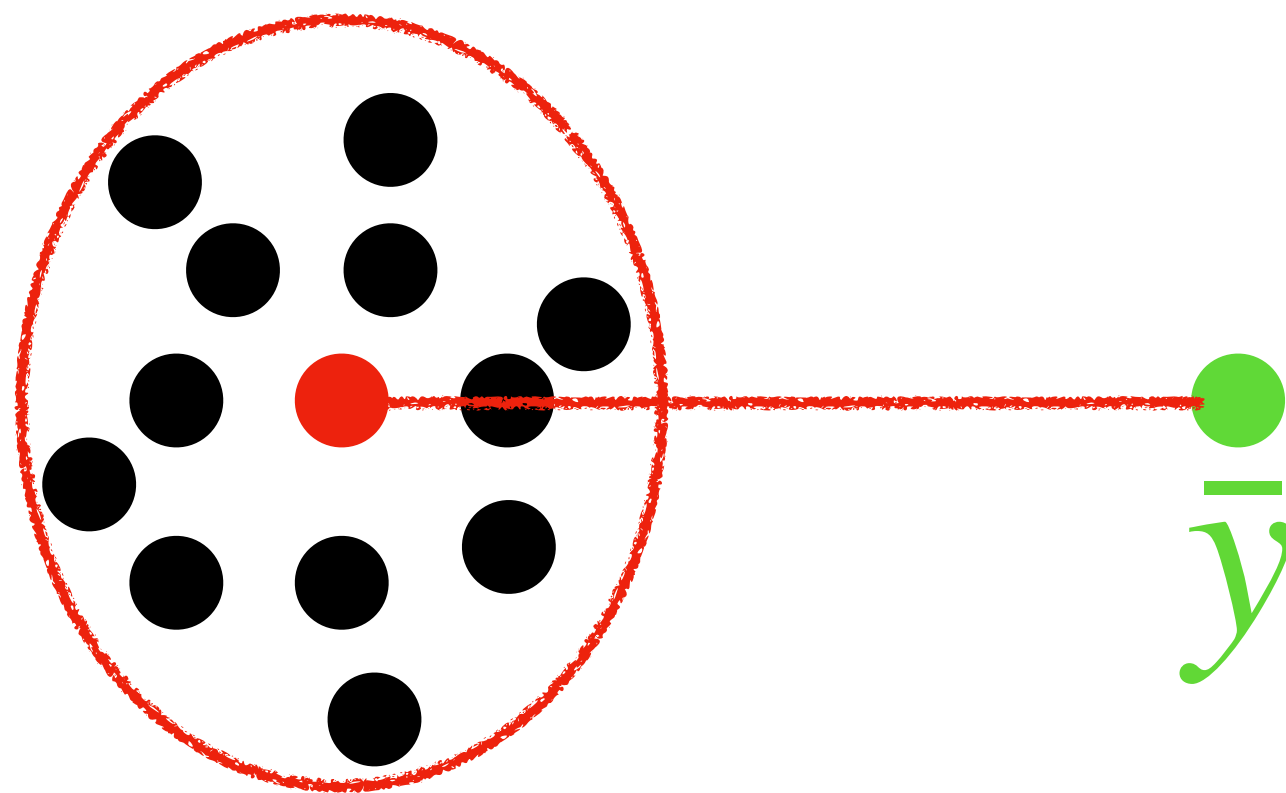
$$\mathbb{E}_{\mathcal{D}, x, y} (h_{\mathcal{D}}(x) - y)^2 = \mathbb{E}_{\mathcal{D}, x} (h_{\mathcal{D}}(x) - \bar{h}(x))^2 + \mathbb{E}_x (\bar{h}(x) - \bar{y}(x))^2 + \mathbb{E}_{x, y} (\bar{y}(x) - y)^2$$

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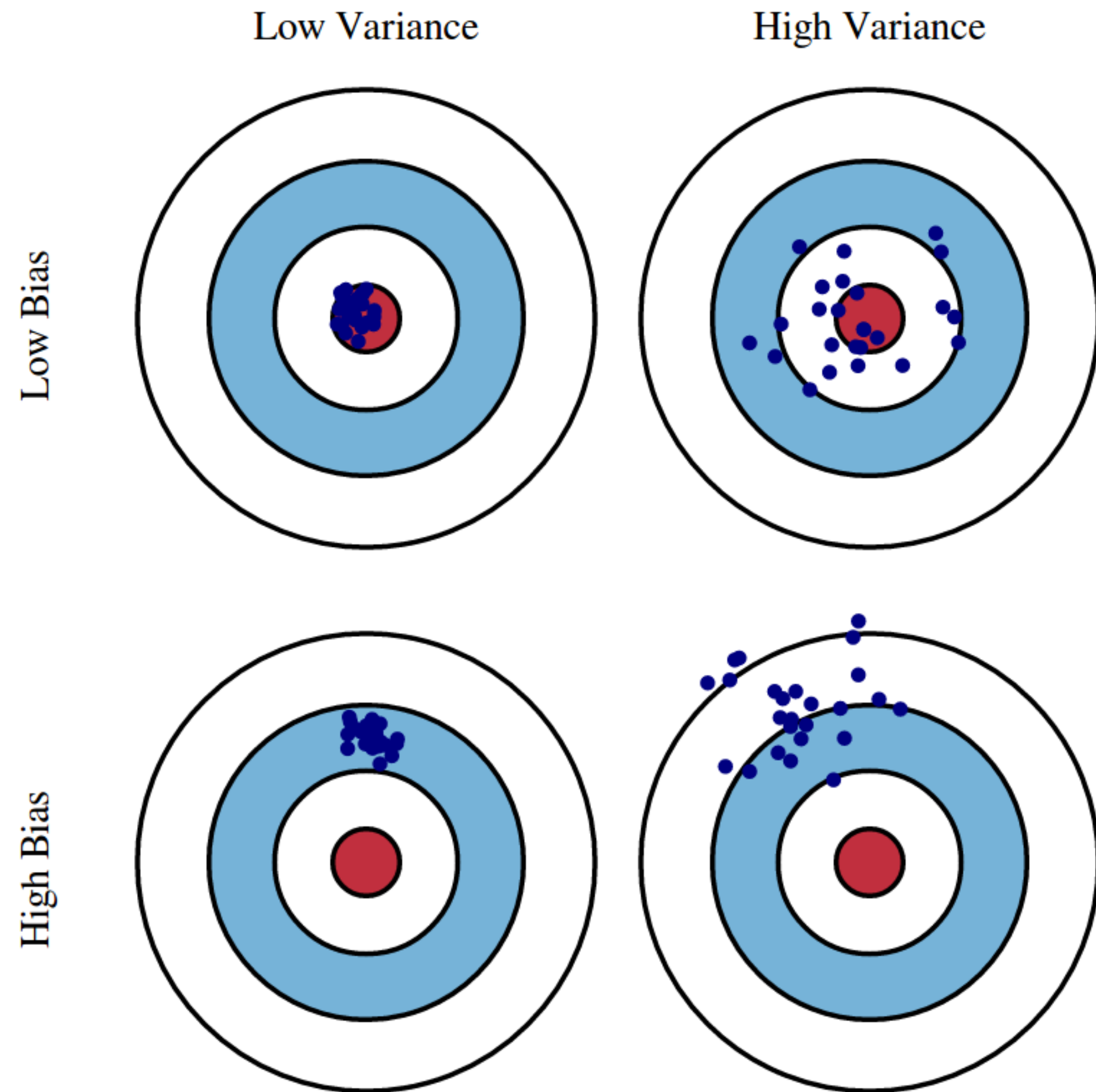
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Recap on Bias-Variance Tradeoff



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 (re-visit Cross Validation)

Ridge Linear regression w/ fixed features and Gaussian noises

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

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

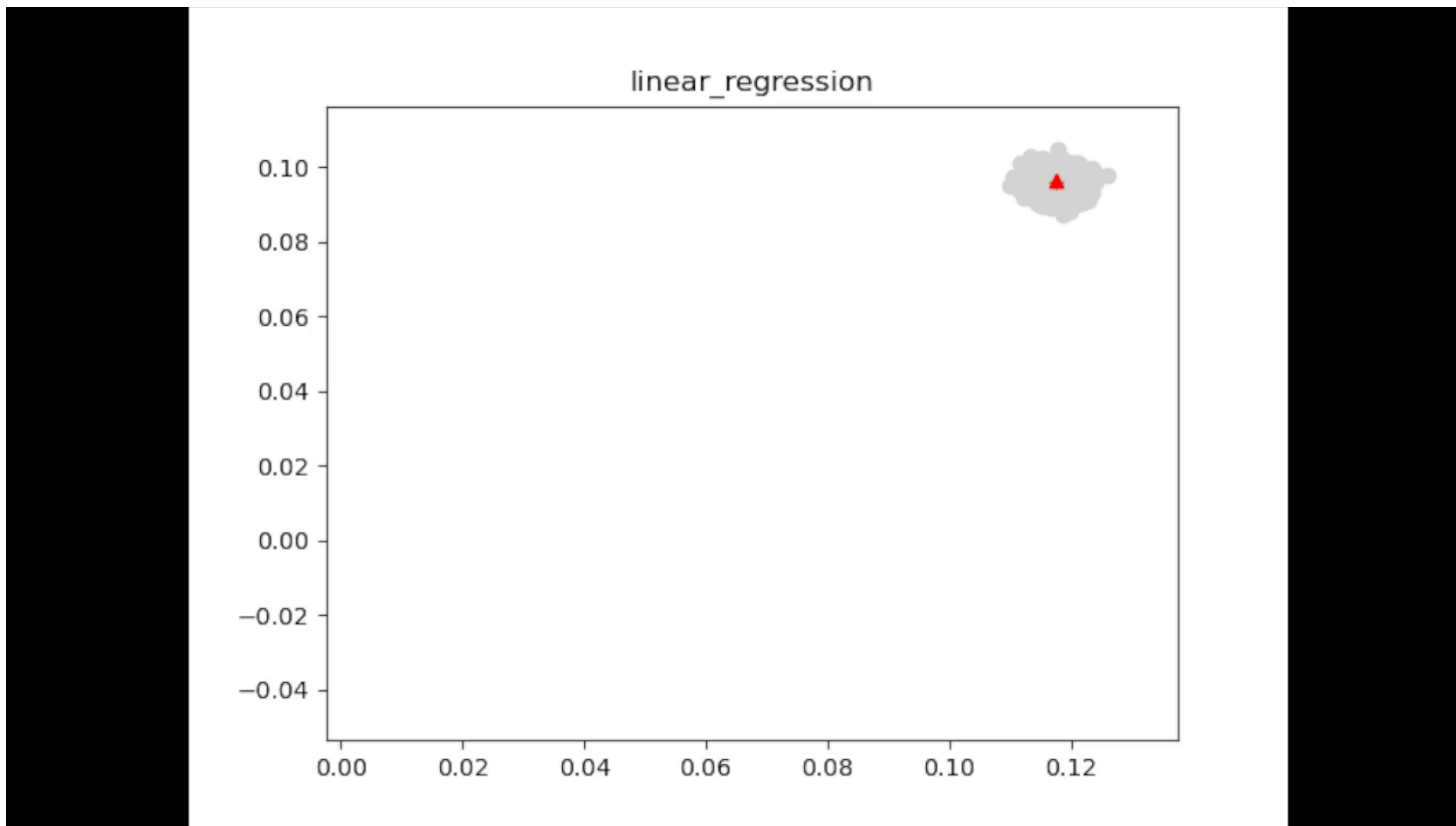
Ridge Linear regression

Demonstration for 2d ridge linear regression

1. We create 5000 datasets: $\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_{5000}$,
2. For a given λ , solve Ridge LR for each dataset, get $\hat{w}_1, \dots, \hat{w}_{5000}$
3. Estimate the mean $\bar{w} = \sum_i \hat{w}_i / 5000$
4. Plot $\hat{w}_1, \dots, \hat{w}_{5000}$, and mean \bar{w} , and the optimal w^\star

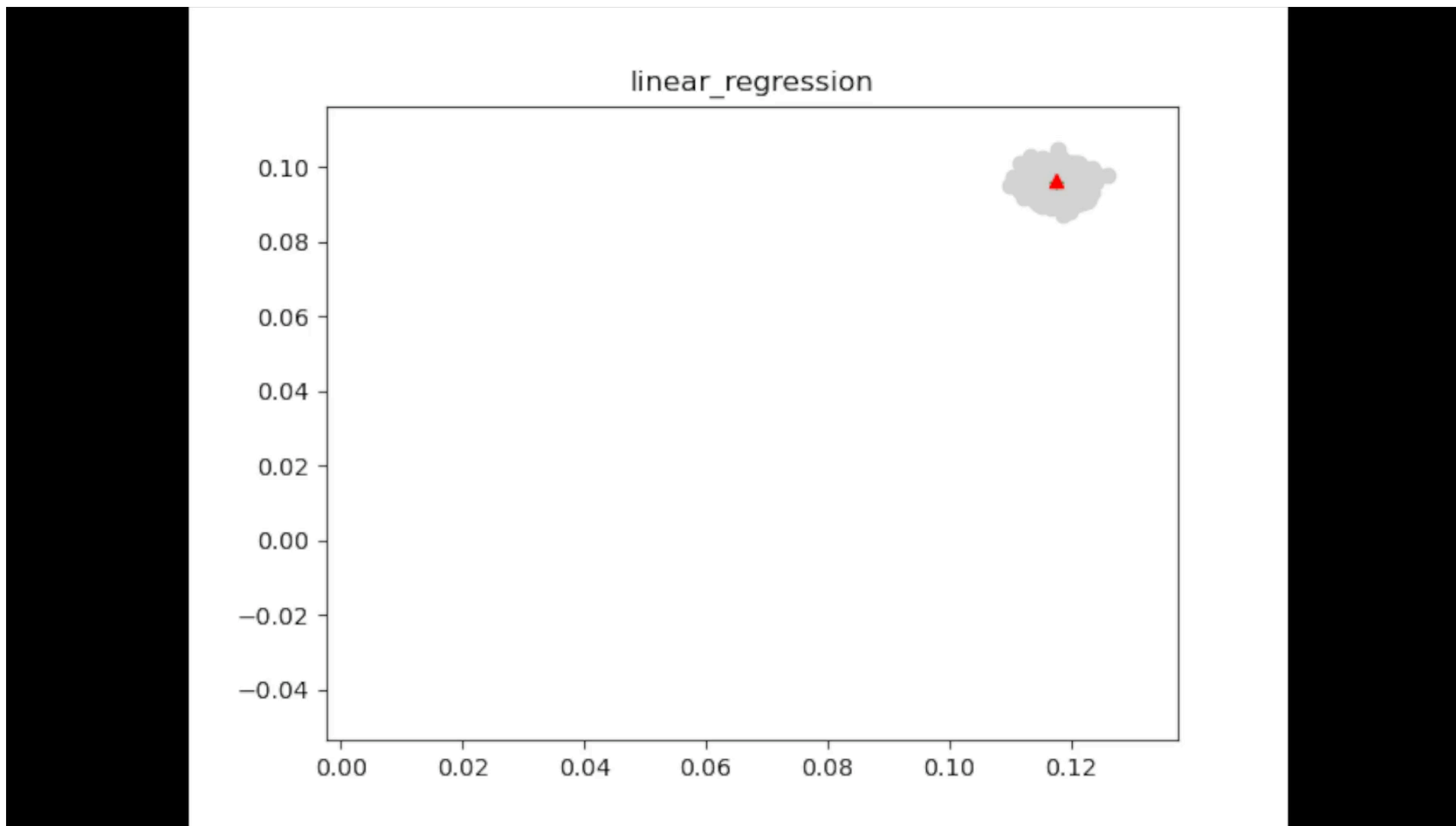
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Derivation of Bias and Variance for Ridge Linear regression

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

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

The Expectation of the Ridge LR solution

Recall we have closed form solution for Ridge LR

$$\hat{w} = (XX^T + \lambda I)^{-1}XY = (XX^T + \lambda I)^{-1}X(X^T w^* + \epsilon)$$

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

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

The Bias of Ridge Linear regression

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

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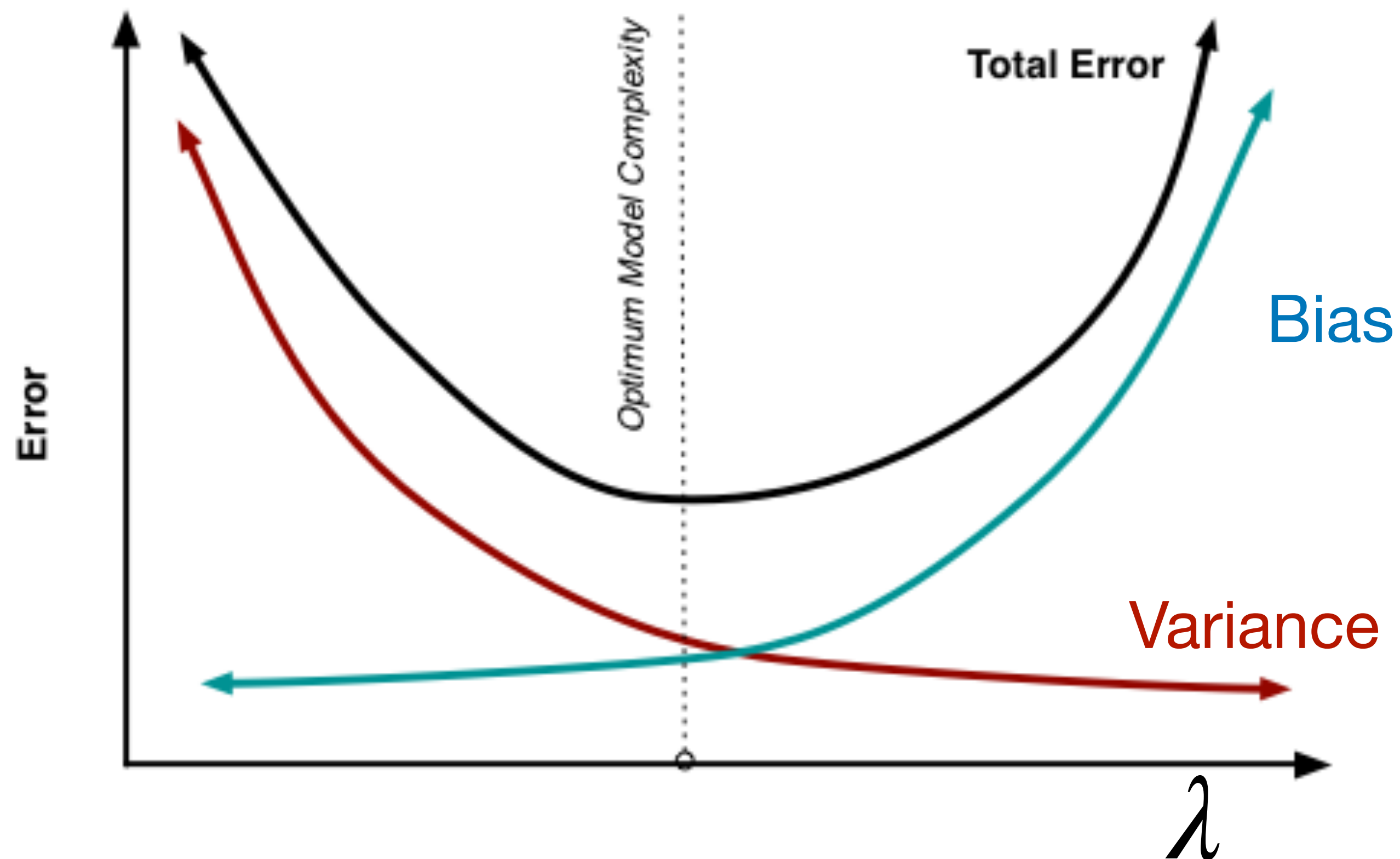
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Ridge Linear regression

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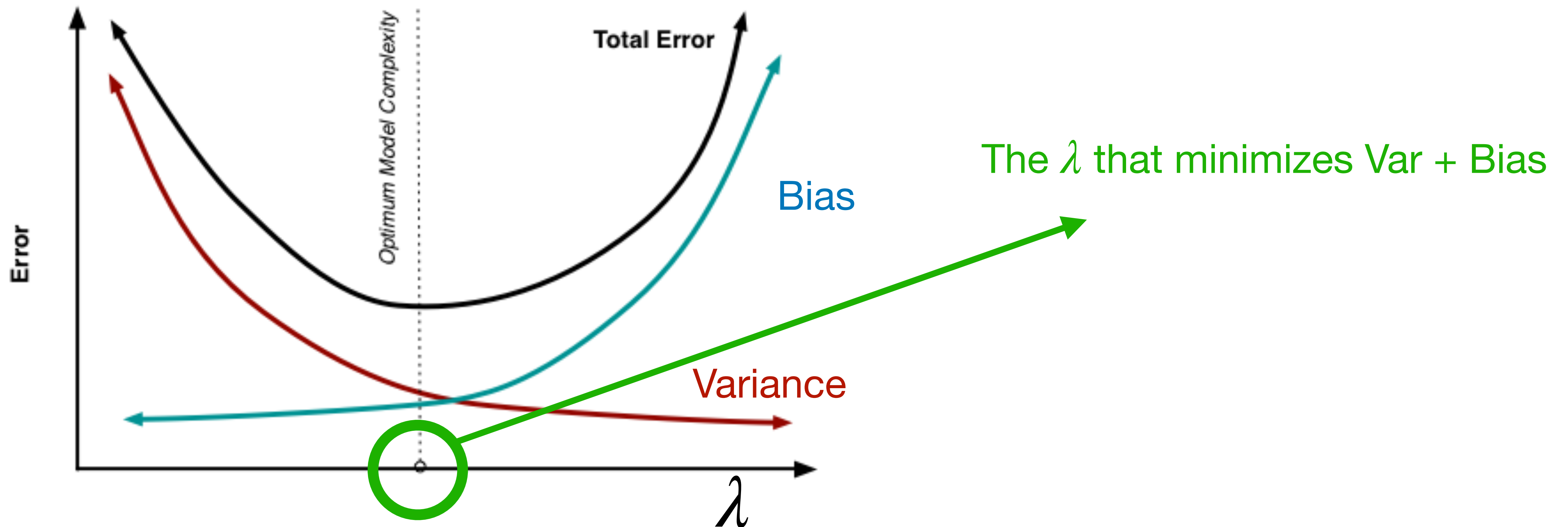
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Cross Validation revisit:

Split the data into K folds

For $i = 1$ to K :

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Generalization error of Ridge LR w/ λ

Output avg validation error $\bar{\epsilon}_\lambda = \sum_{i=1}^K \epsilon_{vad;i} / K$

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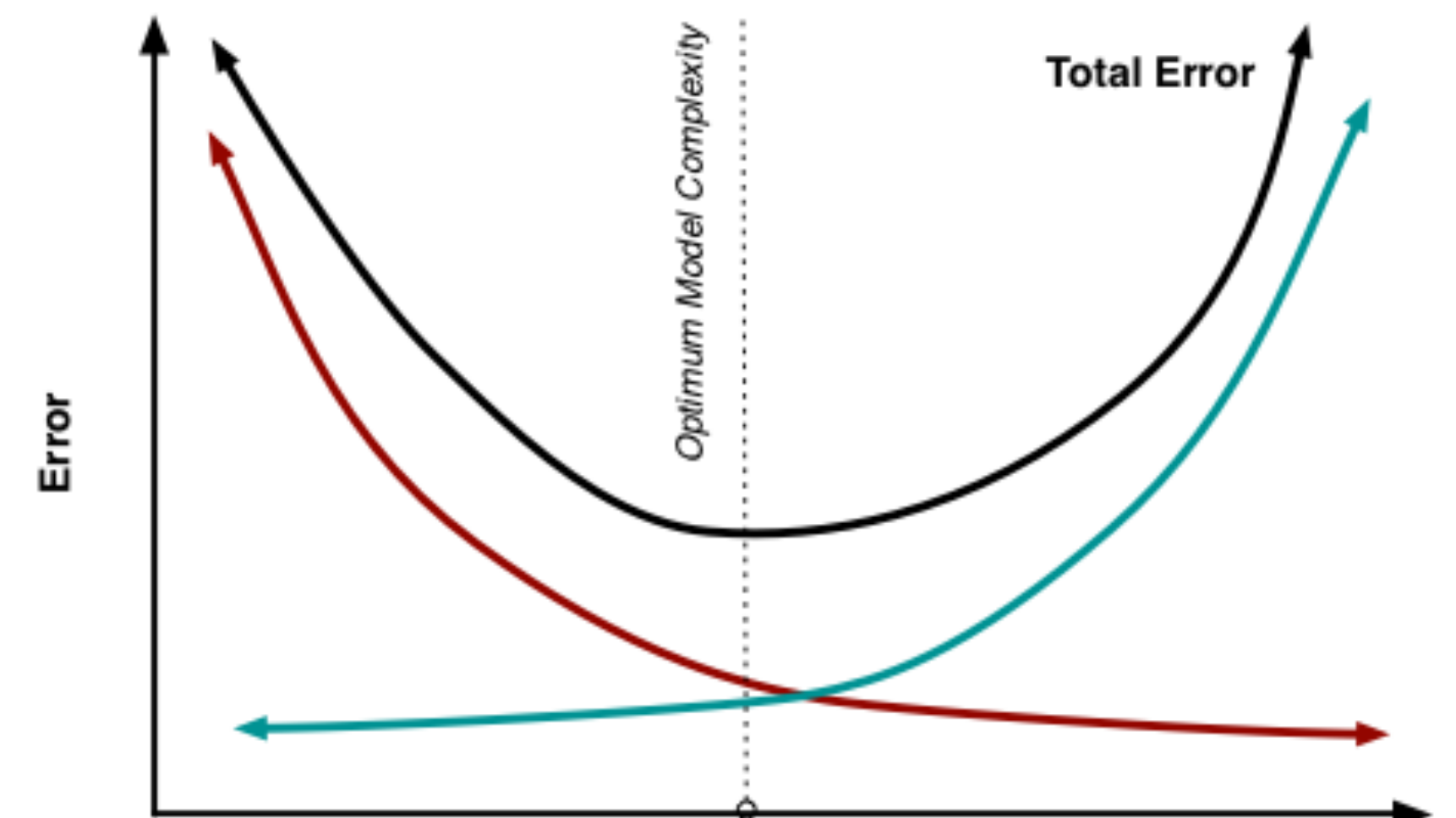
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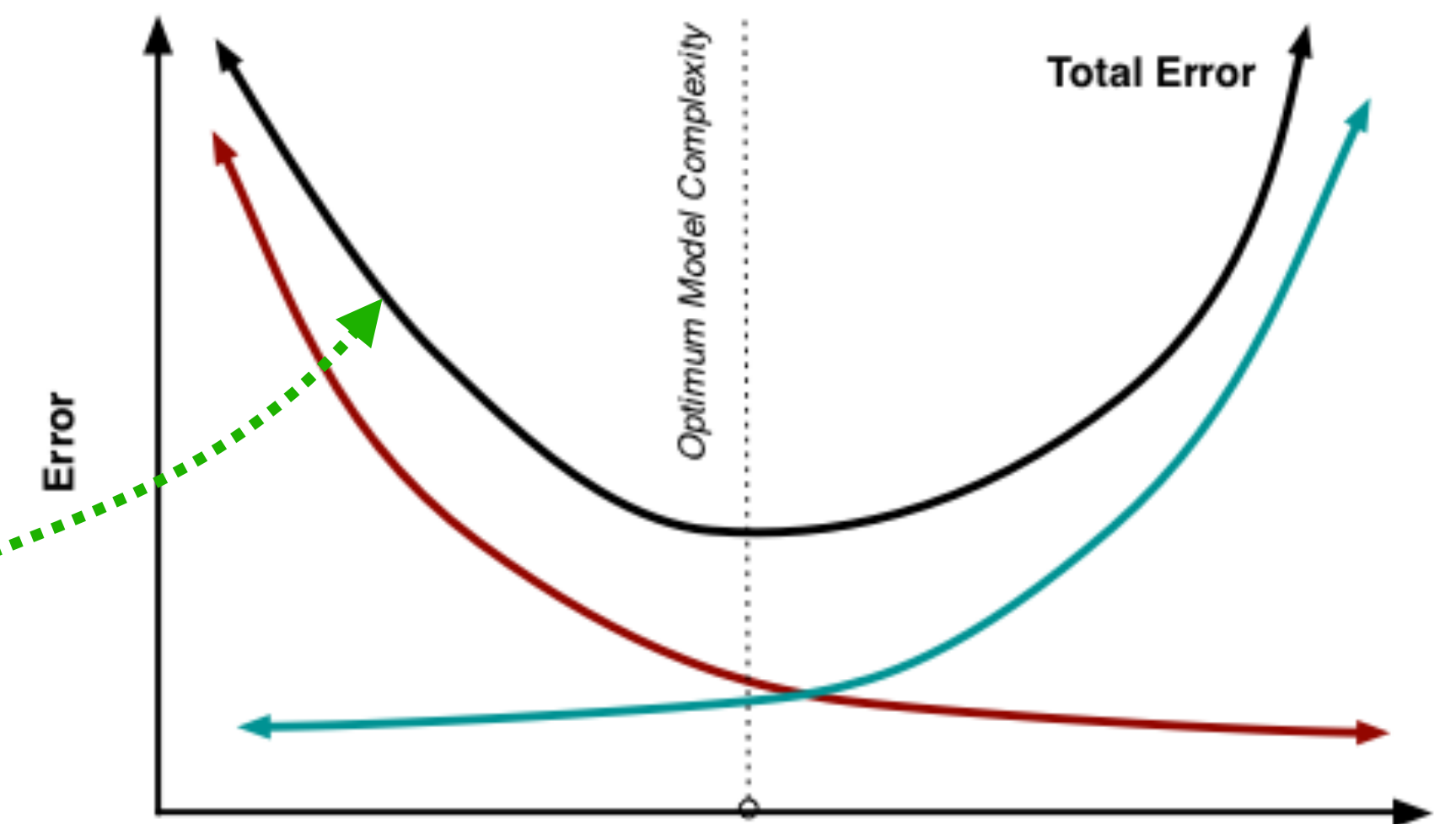
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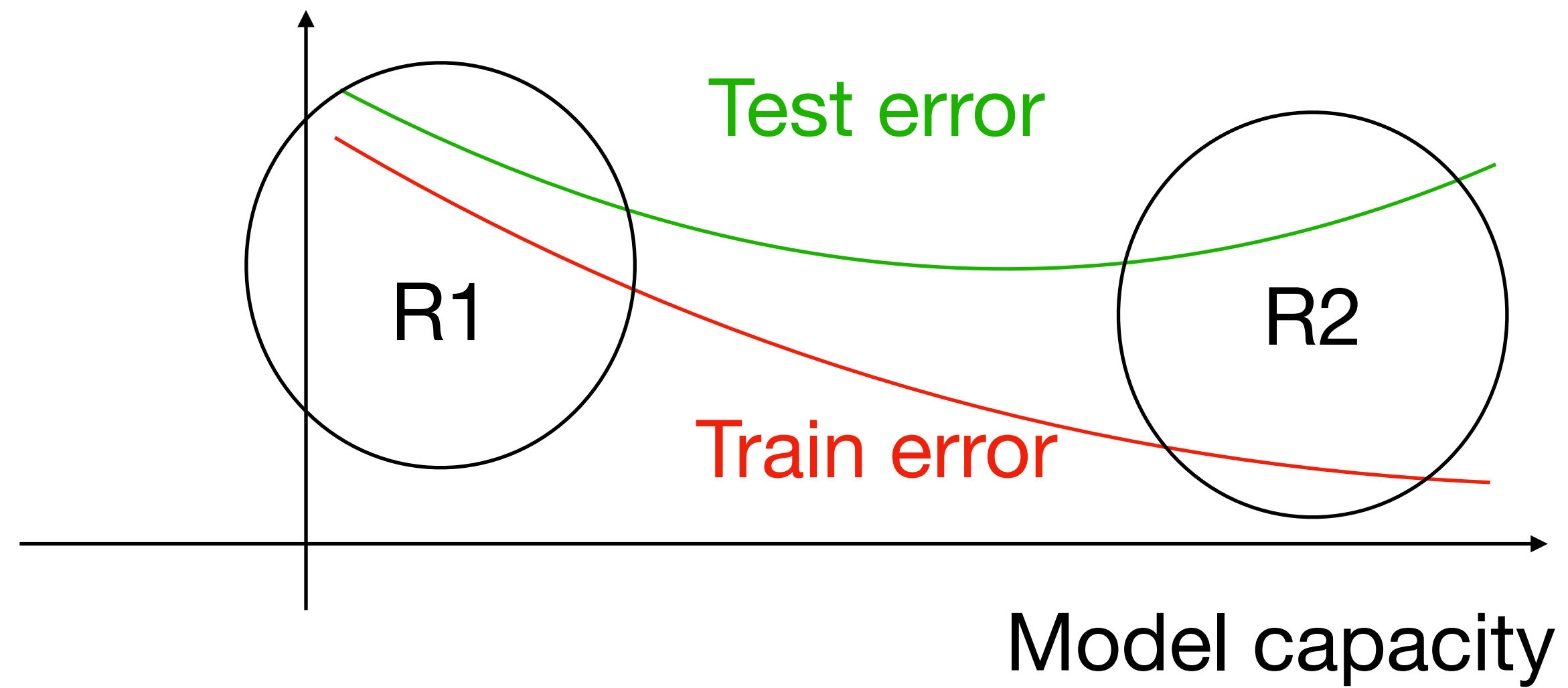
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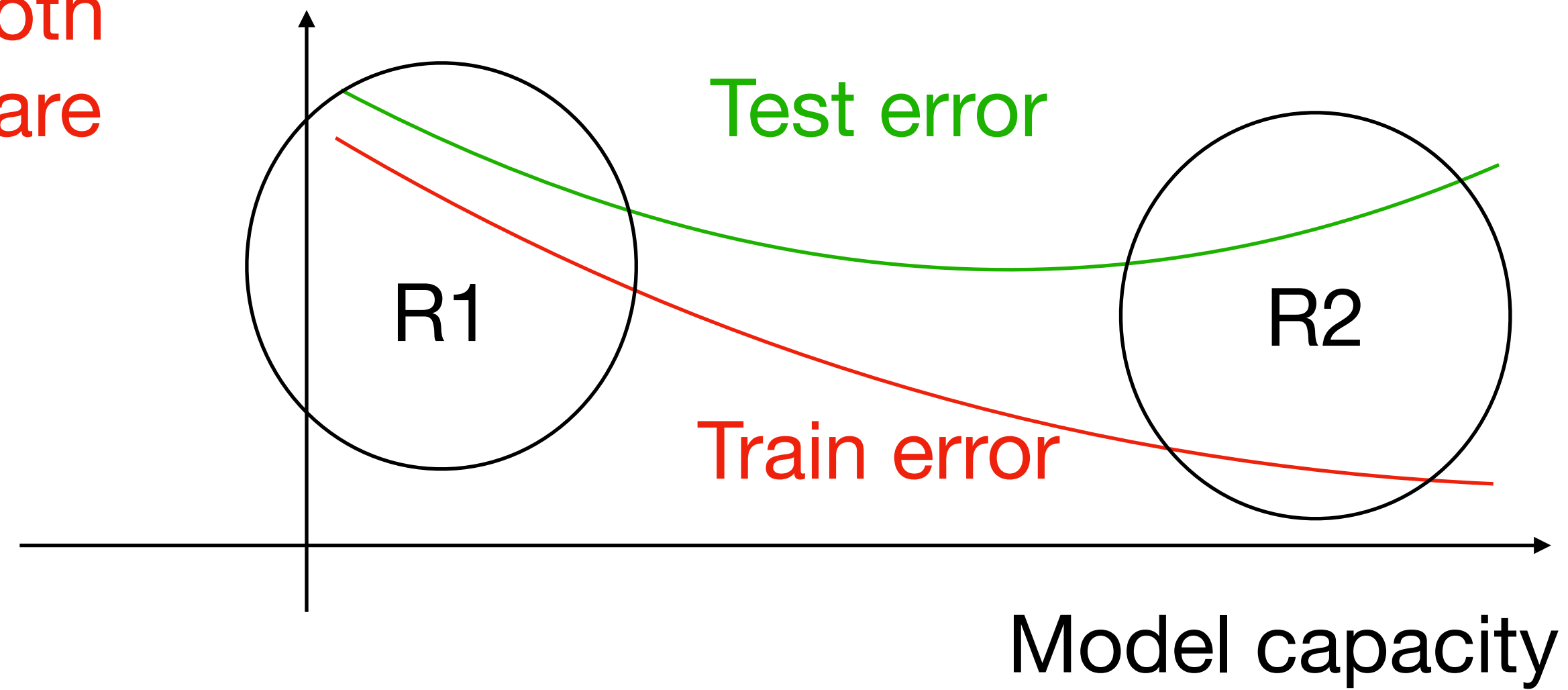
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Practical Suggestions for combating over/under fitting



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

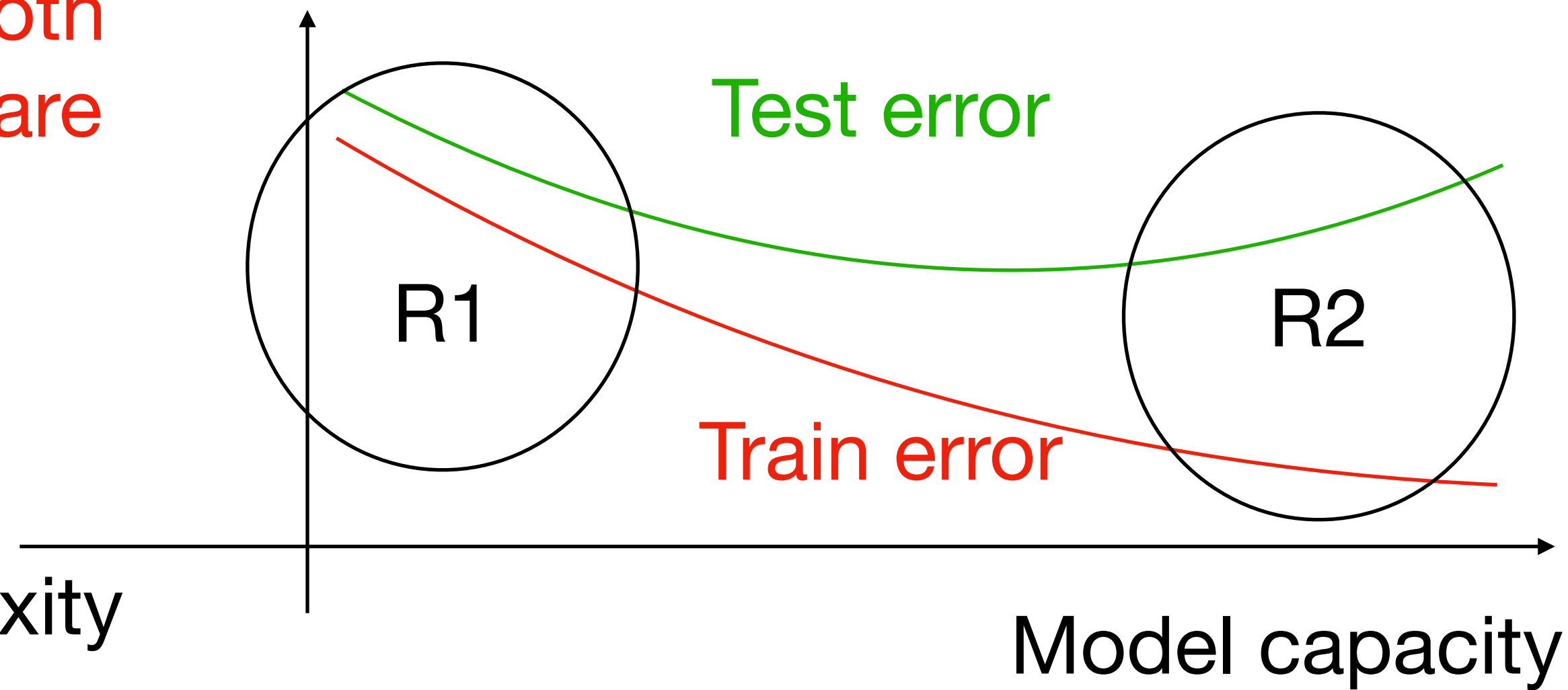


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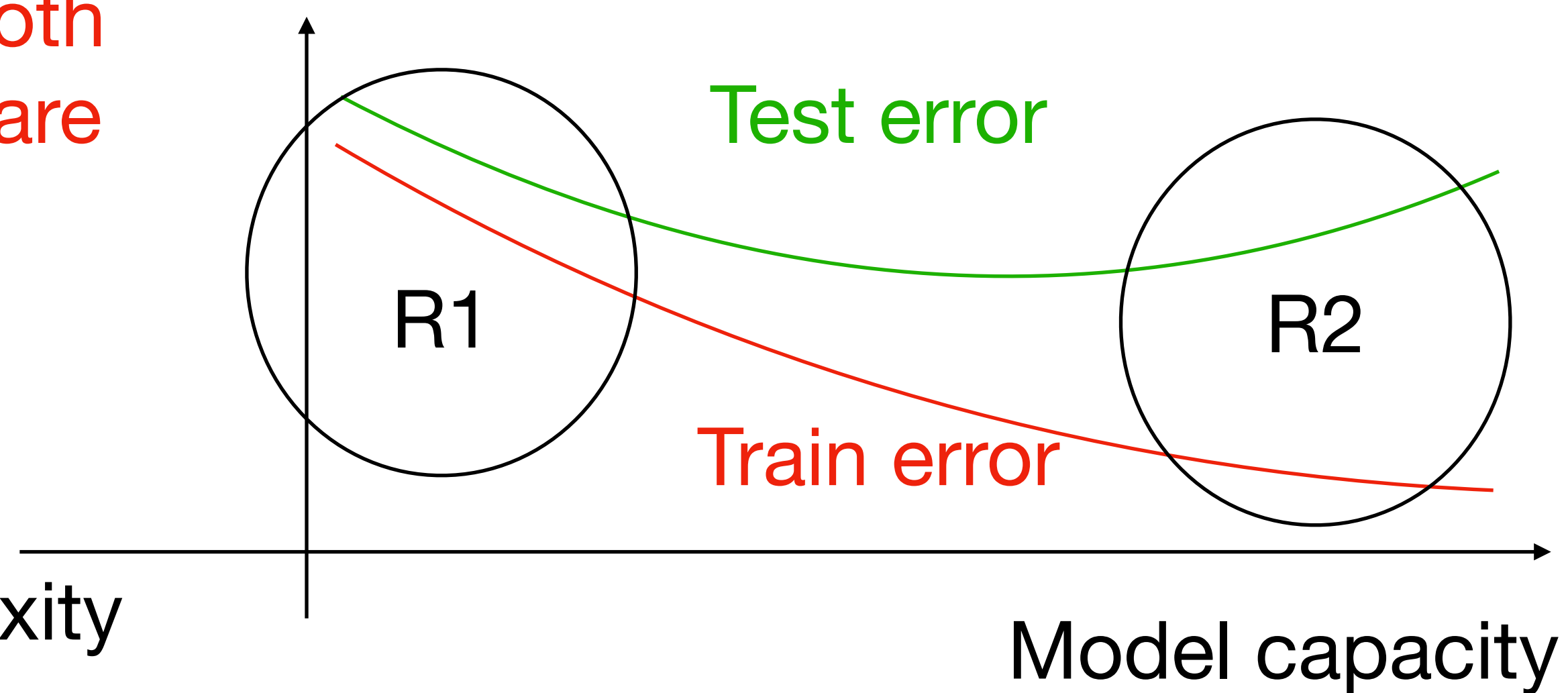


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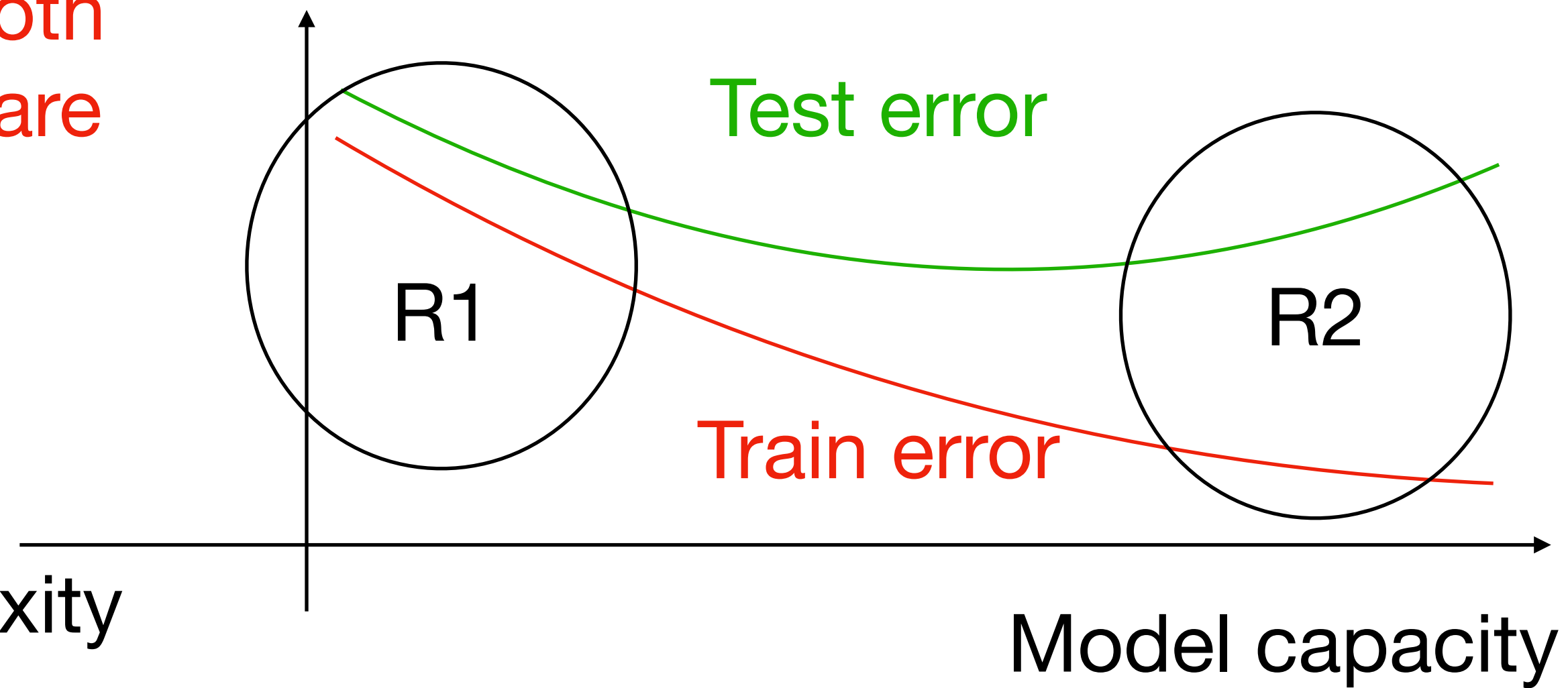


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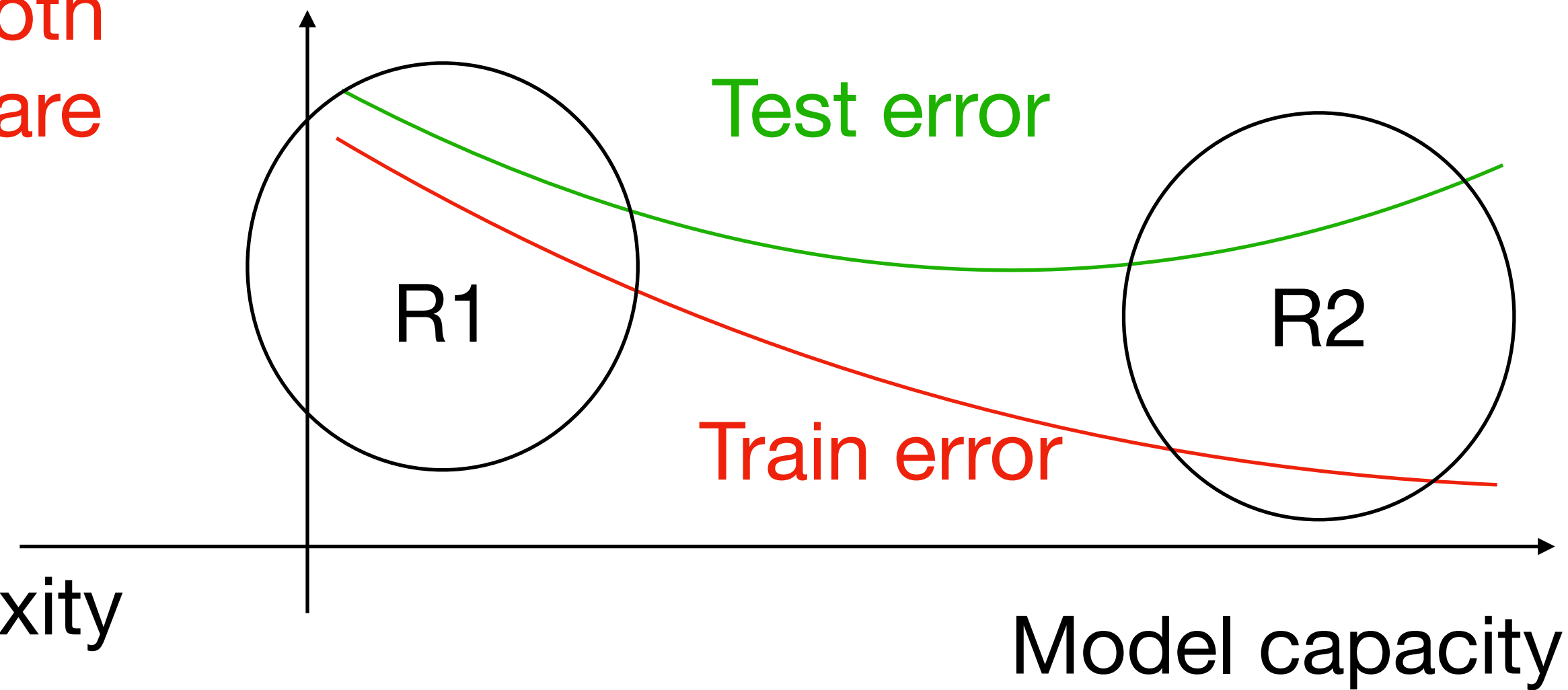


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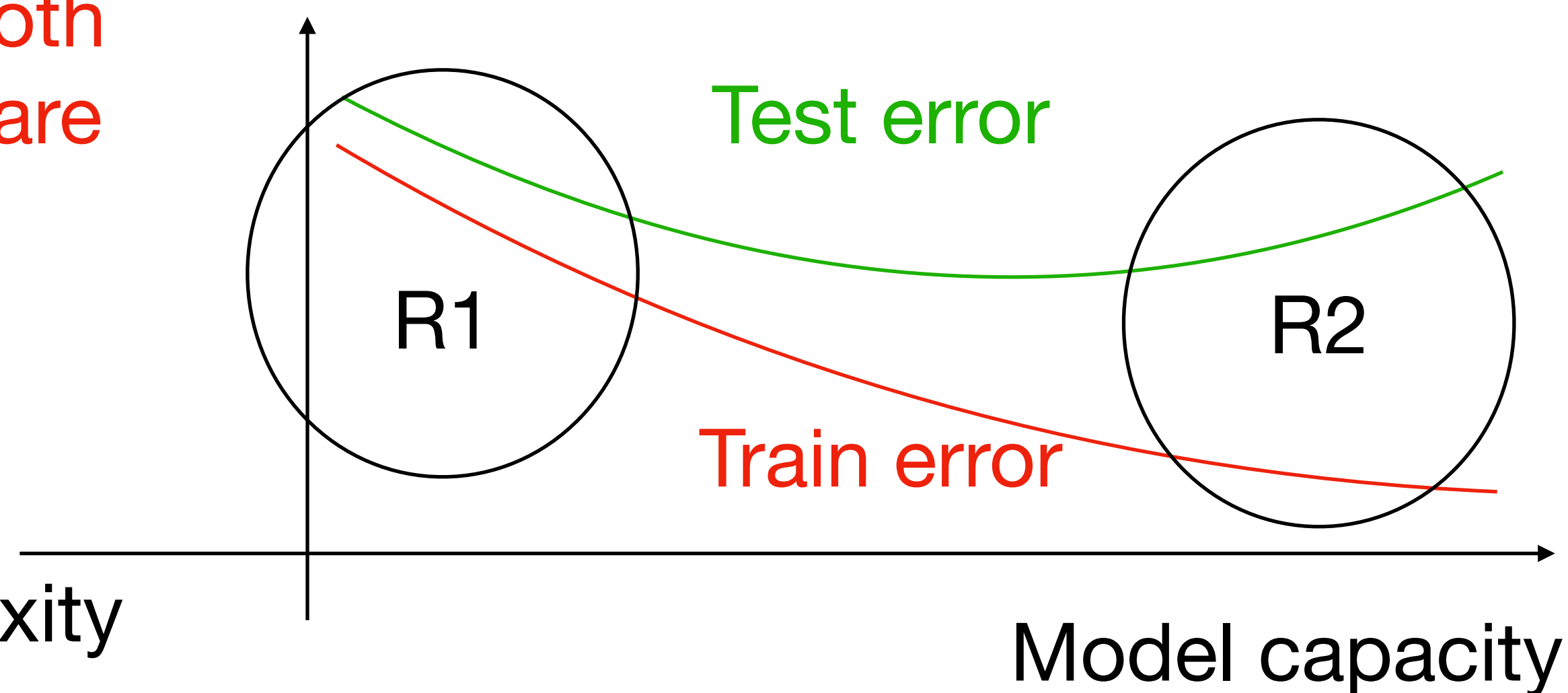
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R2: overfitting (small train err but large test err)

Suggestions:

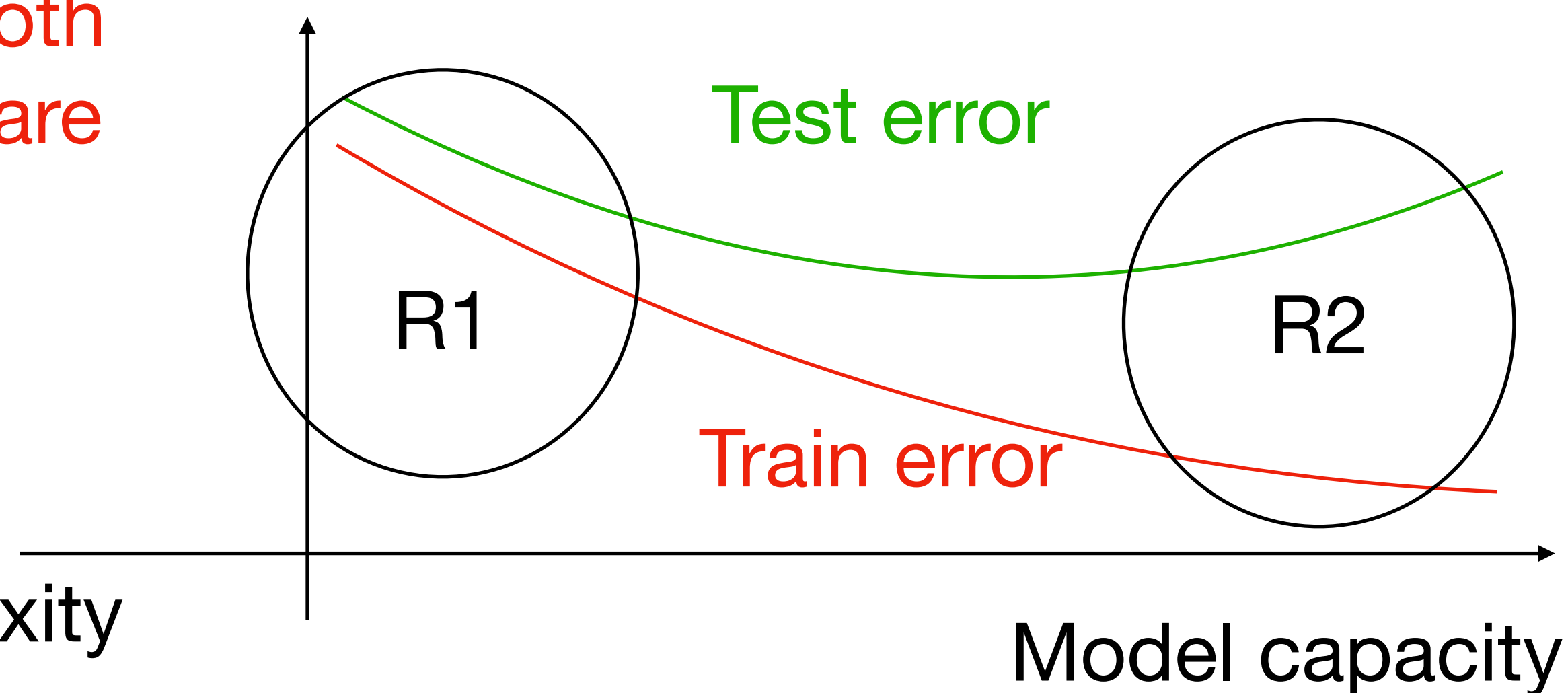
1. More train data

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)



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Suggestions:

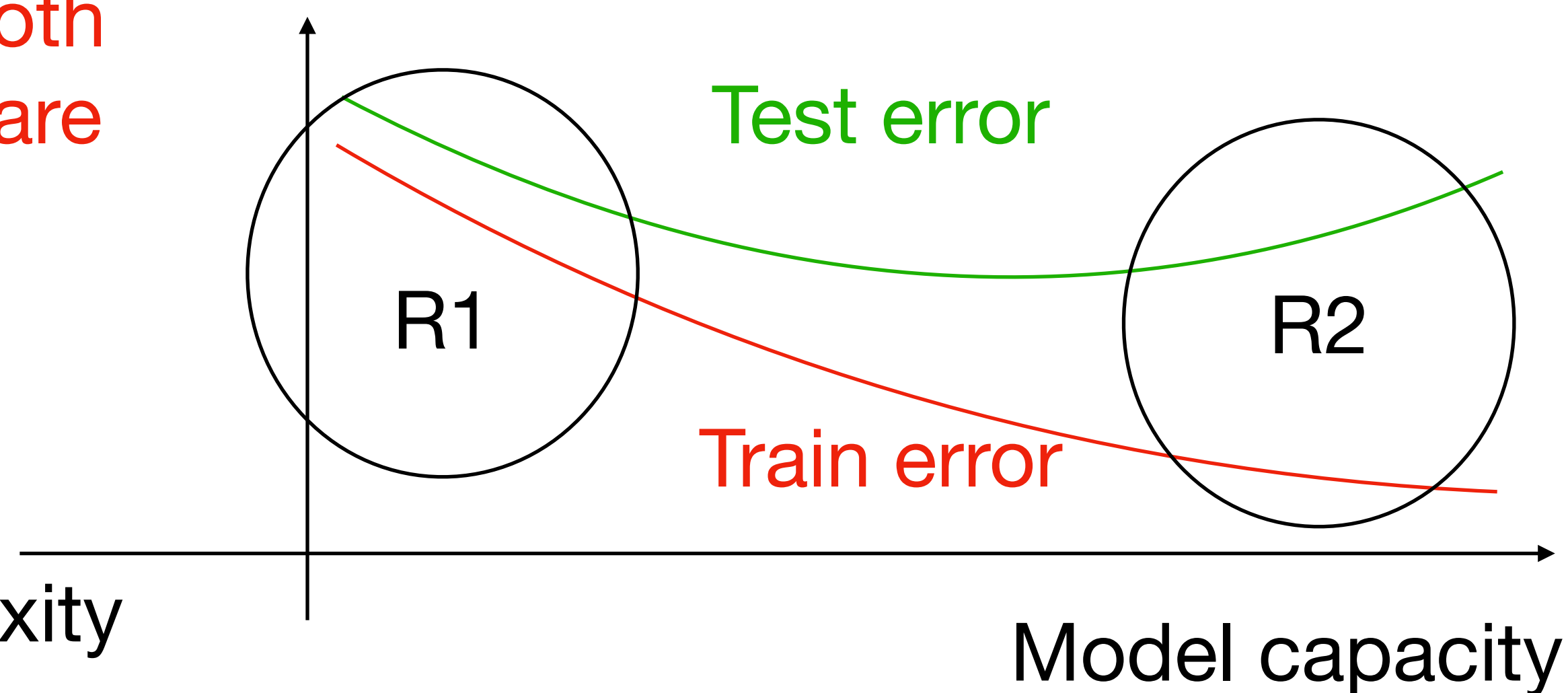
1. More train data
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