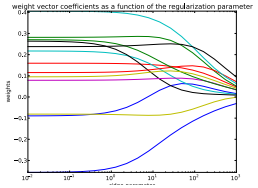
Regularization and model selection

Chapter 4



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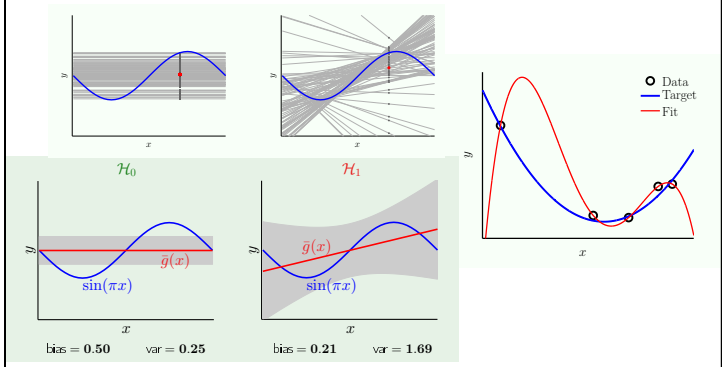
Reminder: bias vs variance, overfitting



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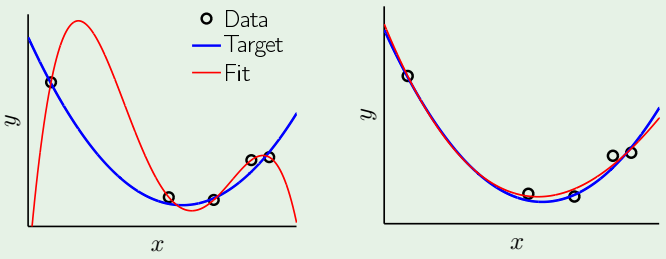
Regularization

The cure for overfitting - regularization



Without regularization

With regularization

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Regularization

How does it work?

- Constrains the model so it cannot fit the noise
- Potential side effect: if it cannot fit the noise, can it fit the target function?
- Introduces bias and reduces variance, so that (hopefully) out-of-sample error is lower

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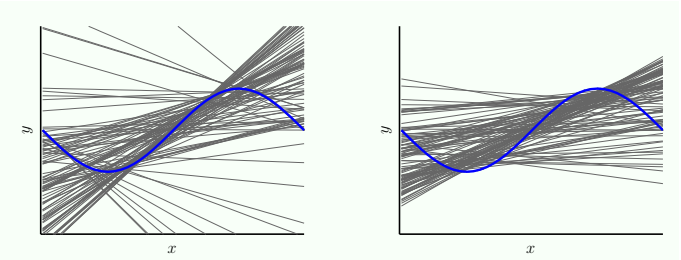
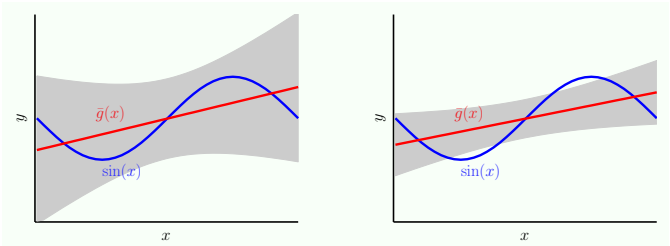
Constraining the model

Let's penalize large weights



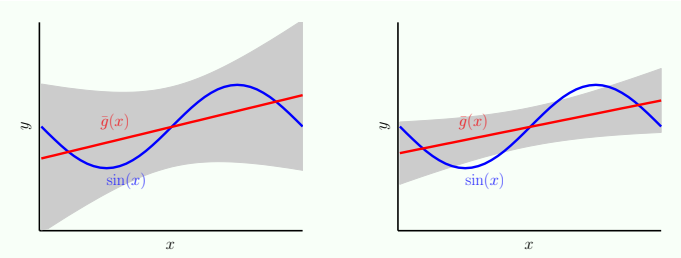
One effect: increased bias



no regularization — bias = 0.21

regularization — bias = 0.23

Second effect: dramatic reduction in variance



no regularization	regularization
bias = 0.21	bias = 0.23
var = 1.69	var = 0.33

Constraining the complexity of the model

Replace E_{in} with:

$$E_{\text{aug}}(h) = E_{\text{in}}(h) + \frac{\lambda}{N}\Omega(h)$$

Regularization term

λ regularization constant

E_{aug} is a better proxy for E_{out} than E_{in}

Choosing a regularizer

We want to constrain the learned function in the direction of the target function.

Intuition: noise is non-smooth

Common choice for the augmented in-sample-error:

$$E_{aug}(\mathbf{w}) = E_{in}(\mathbf{w}) + \lambda \mathbf{w}^\intercal \mathbf{w}$$

weight decay regularizer

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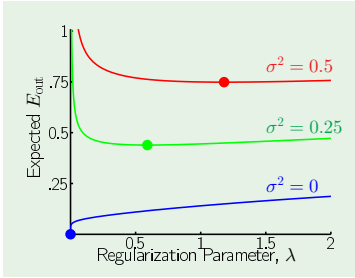
Is there an optimal value for λ?

The behavior of E_{out} as a function of the regularization parameter for varying levels of noise:



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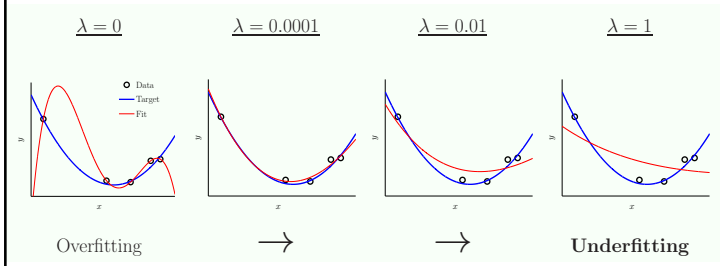
Is there an optimal value for λ?

Minimizing $E_{aug}(\mathbf{w}) = E_{in}(\mathbf{w}) + \lambda \mathbf{w}^\intercal \mathbf{w}$



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Regularized least-squares

Ridge regression:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \ (\mathbf{y} - \mathbf{X}\mathbf{w})^\intercal (\mathbf{y} - \mathbf{X}\mathbf{w}) + \lambda ||\mathbf{w}||^2$$
$$= (\mathbf{X}^\intercal \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\intercal \mathbf{y}$$

The regularization term controls the size of the components of the weight vector.

There is a tradeoff between fitting (the error term) and regularization. The regularization terms can therefore prevent overfitting. The parameter λ controls this tradeoff.

Many ML methods can be expressed as solution to a criterion of the form:

error term + regularization term

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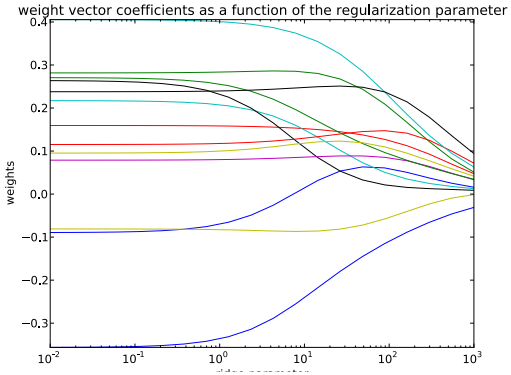
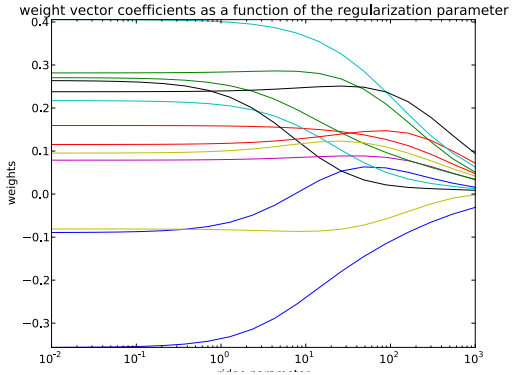
The effect of the regularization parameter



Each curve is the magnitude of the weight vector associated with a given feature. Computed on the scaled version of the "heart" dataset.

The effect of the regularization parameter



As the regularization parameter increases, w_i shrinks toward 0

Assignment 3

Explore the effect of regularization with least-squares regression.

The validation set

How to choose the value of the regularization parameter?

Take a sneak peak at E_{out} using a validation set!

On a validation set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_K, y_K)$, the error is $E_{\text{val}}(h) = \frac{1}{K} \sum_{k=1}^{K} \mathbf{e}(h(\mathbf{x}_k), y_k)$

$$\mathbb{E}\left[E_{\text{val}}(h)\right] = \frac{1}{K} \sum_{k=1}^{K} \mathbb{E}\left[\mathbf{e}(h(\mathbf{x}_k), y_k)\right] = E_{\text{out}}(h)$$

$$\text{var}\left[E_{\text{val}}(h)\right] = \frac{1}{K^2} \sum_{k=1}^{K} \text{var}\left[\mathbf{e}(h(\mathbf{x}_k), y_k)\right] = \frac{\sigma^2}{K}$$

$$E_{\text{val}}(h) = E_{\text{out}}(h) \pm O\left(\frac{1}{\sqrt{K}}\right)$$

Section 4.3.1

Choosing the size of the validation set

Given the data set $\mathcal{D} = (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$

$\underbrace{K \text{ points}}_{\mathcal{D}_{\text{val}}} \rightarrow$ validation $\quad \underbrace{N-K \text{ points}}_{\mathcal{D}_{\text{train}}} \rightarrow$ training

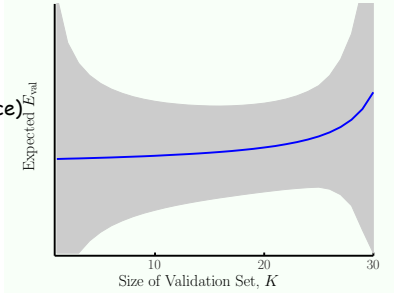
$O\left(\frac{1}{\sqrt{K}}\right)$: Small $K \implies$ bad estimate

Large $K \implies$?

Rule of thumb: use 20% of the data for validation

Choosing the size of the validation set

Shaded region:
the uncertainty (variance)
of the estimate

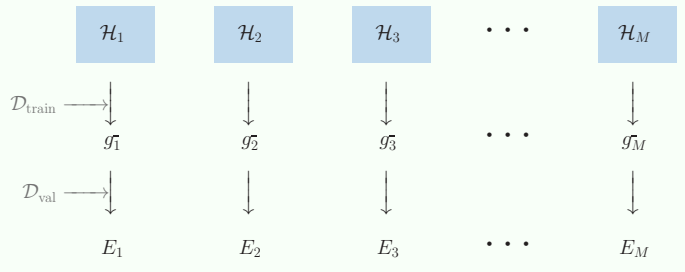


Observations:

- As we increase the size of the validation set, the estimate goes up because of a small training set
- The uncertainty in E_{val} decreases as we increase K, up to a point, where a small training set size generates uncertainty in the estimate

Using the validation set

The validation set is used to get estimates that allow us to choose a value for the regularization parameter.



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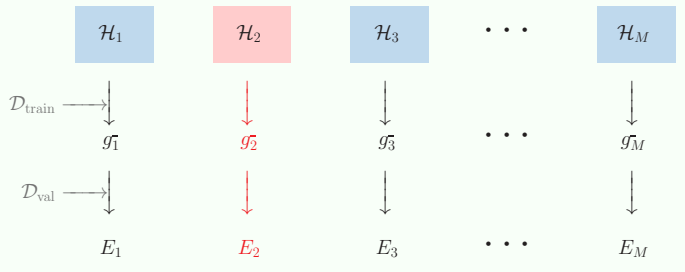


Using the validation set

The validation set is used to get estimates that allow us to choose a value for the regularization parameter.

$(\mathcal{H}, \lambda_1)$ $(\mathcal{H}, \lambda_2)$ $(\mathcal{H}, \lambda_3)$ $\cdots$ $(\mathcal{H}, \lambda_M)$

$\downarrow$ $\downarrow$ $\downarrow$ $\cdots$ $\downarrow$

g_1 g_2 g_3 $\cdots$ g_M

Using the validation set

M models $\mathcal{H}_1, \ldots, \mathcal{H}_M$

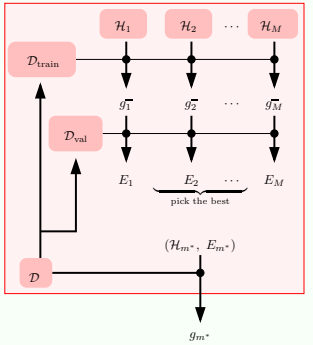
Use $\mathcal{D}_{\text{train}}$ to learn g_m^- for each model

Evaluate g_m^- using $\mathcal{D}_{\text{val}}$:

$$E_m = E_{\text{val}}(g_m^-); \quad m = 1, \ldots, M$$

Pick model $m = m^*$ with smallest E_m

At the end: train a model on all the data using the parameters of H_{m^*}.



We have a dilemma...

We would like to have the following:

$$E_{\text{out}}(g) \approx E_{\text{out}}(g^-) \approx E_{\text{val}}(g^-)$$

(small K) (large K)

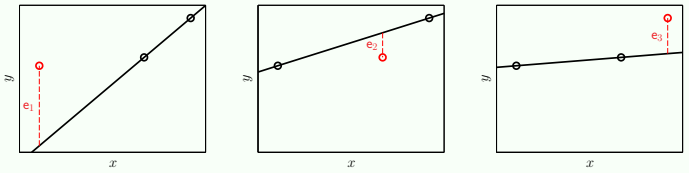
g : the model as a result of training on all the data

g^-: the model trained on D_{train}

Can we have K both large and small?

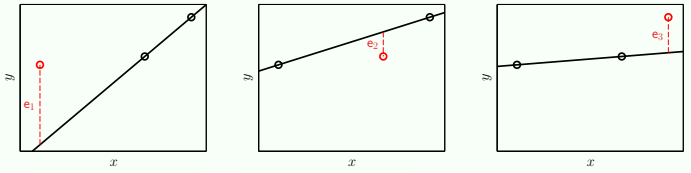
Leave-one-out errors

Extreme case: K=1



The leave-one-out estimate

Extreme case: K=1



$\mathbb{E}[e_1] = E_{\text{out}}(g_1^-)$

$E_{\text{cv}} = \frac{1}{N}\sum_{n=1}^{N} e_n$

Theorem. E_{cv} is an unbiased estimate of $\bar{E}_{\text{out}}(N-1)$.

Expected E_{out} when learning with $N-1$ points.

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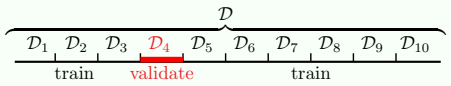
Cross validation

The leave-one-out estimate is expensive to compute!

Cross validation:

- Randomly partition the data into k parts ("folds").
- Set one fold aside for evaluation and train a model on the remaining k-1 folds and evaluate it on the held-out fold.
- Repeat until each fold has been used for evaluation



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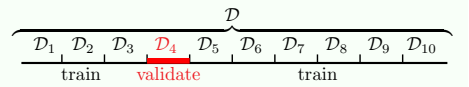

- The reported error is the average over the errors for each fold.

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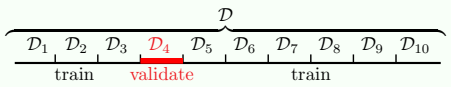

Stratified-cross validation aims at achieving roughly the same class distribution in each fold.

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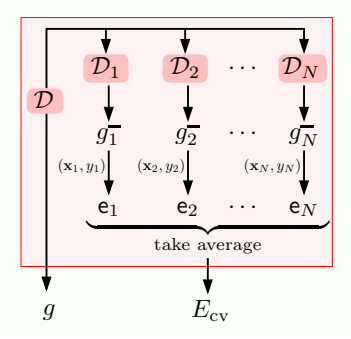
Using cross-validation



customer

select the best model

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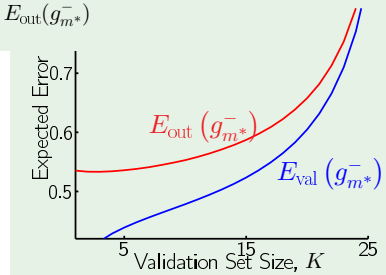
Bias

The error estimates using the validation set are optimistic estimates of E_{out}!

We selected the model $\mathcal{H}_{m^*}$ using $\mathcal{D}_{\text{val}}$

$E_{\text{val}}(g_{m^*}^-)$ is a biased estimate of $E_{\text{out}}(g_{m^*}^-)$



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Bias

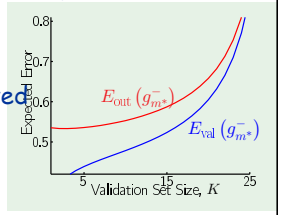
The error estimates using the validation set are optimistic estimates of E_{out}!

We selected the model $\mathcal{H}_{m^*}$ using $\mathcal{D}_{\text{val}}$

$E_{\text{val}}(g_{m^*}^-)$ is a biased estimate of $E_{\text{out}}(g_{m^*}^-)$

So you need to have a separate test set.

Training set: totally contaminated
Validation set: slightly contaminated
Test set: "clean"



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Measures of classifier performance

Classifier performance can be summarized by a table known as the confusion matrix or contingency table:

true labels	predicted labels:	
	-1	1
-1	1439	61
1	62	1438

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Measures of classifier performance

Let's take a closer look at the contingency table:

true labels	predicted labels:	
	-1	1
-1	1439	61
1	62	1438

How do we compute error from the contingency table?

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Measures of classifier performance

For binary classification problems it is customary to express the contingency table as:

true labels	predicted labels:	
	-1	1
-1	TN	FP
1	FN	TP

TP – number of true positives
TN – number of true negatives
FP – number of false positives
FN – number of false negatives

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Measures of classifier performance

For binary classification problems it is customary to express the contingency table as:

true labels	predicted labels:		
	-1	1	
-1	TN	FP	Neg = TN+FP
1	FN	TP	Pos = TP+FN

True positive rate/sensitivity/recall: TP / Pos
True negative rate/specificity: TN / Neg
False positive rate: FP / Neg
Precision: TP / (TP + FP)

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Measures of classifier performance

Suppose you have a dataset with very few positive examples compared to negative examples (unbalanced data)

A classifier that classifies every example as negative would still attain high accuracy (this is called the majority class classifier).

Need an alternative measure of accuracy!

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The choice of classification threshold

All the classifiers we will study provide a scoring function whose magnitude indicates how sure we are it belongs to a given class. For example: $\mathbf{w}^T\mathbf{x} + b$

The choice of the threshold is somewhat arbitrary, and in a given application we may prefer to ignore positive predictions that are associated with small scores

To have a view of classifier performance that is independent of the choice of threshold we consider the ROC curve.

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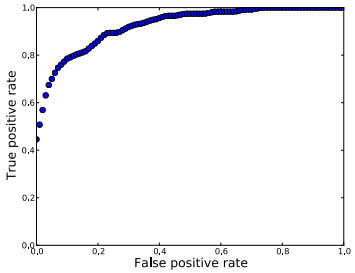
ROC curve

The ROC curve is a plot of the true positive rate as a function of false positive rate as you vary the classification threshold



How does the ROC curve of a perfect classifier look like?

For a random classifier?

ROC curve computed on the heart disease dataset from the UCI repository

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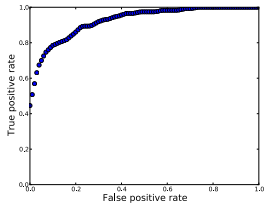
ROC curves and ranking

An ROC curve is often summarized by the area under the curve (AUC).

AUC = 0.92



AUC is essentially the probability that a positive example will get a higher score than a negative example

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ROC curves

This is also a nice way of comparing classifiers: