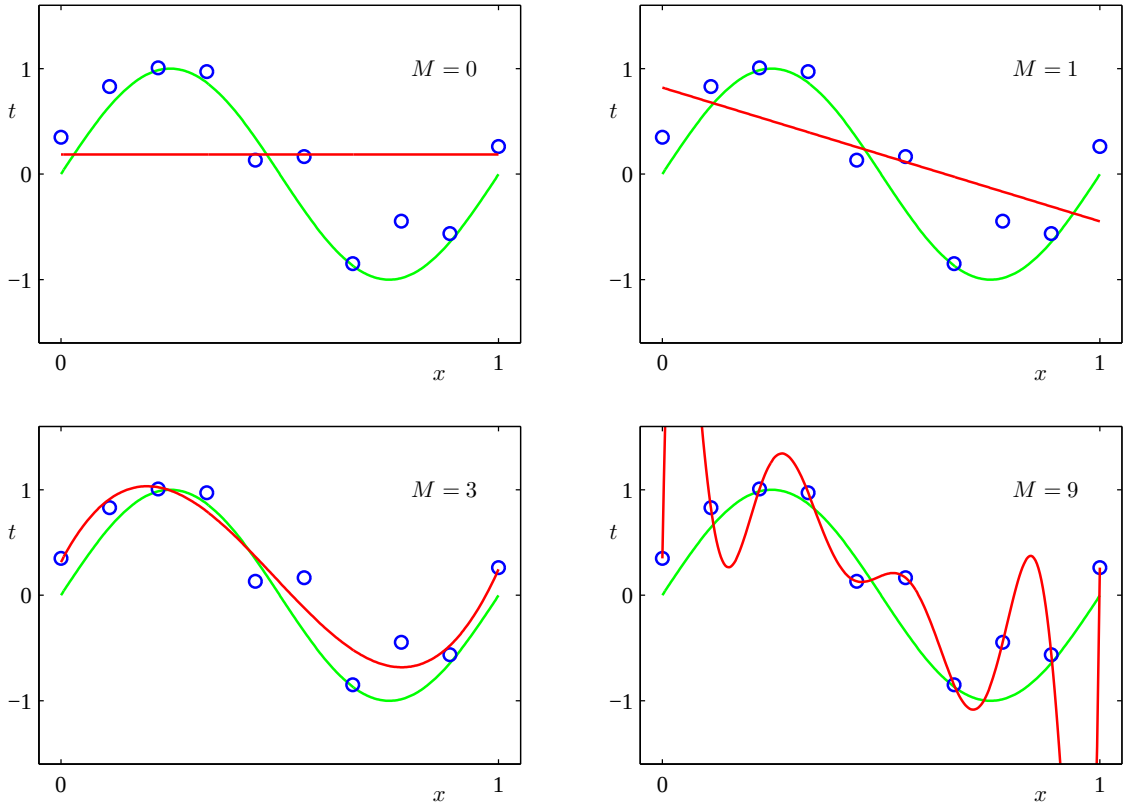
Lecture 2: Overfitting. Regularization

- Overfitting
- Cross-validation
- L2 and L1 regularization for linear estimators
- Bias-variance trade-off

Recall: Overfitting

- A general, *HUGELY IMPORTANT* problem for all machine learning algorithms
- We can find a hypothesis that predicts perfectly the training data but *does not generalize* well to new data
- E.g., a lookup table!

Another overfitting example

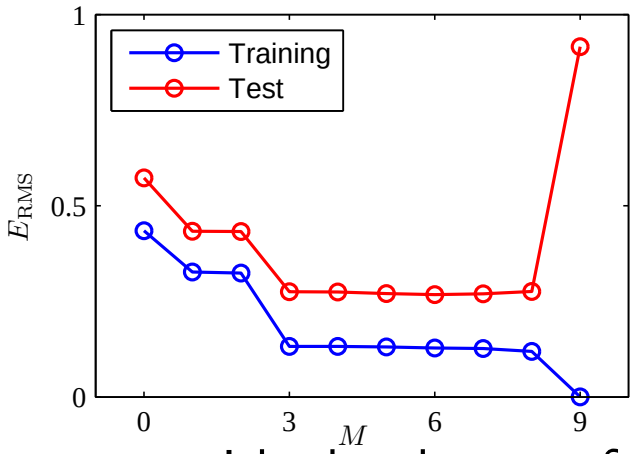


- The higher the degree of the polynomial M, the more degrees of freedom, and the more capacity to "overfit" the training data
- Typical overfitting means that error on the training data is very low, but error on new instances is high

Overfitting more formally

- Assume that the data is drawn from some fixed, unknown probability distribution
- Every hypothesis has a "true" error $J^*(h)$, which is the expected error when data is drawn from the distribution.
- Because we do not have all the data, we measure the error on the training set $J_D(h)$
- Suppose we compare hypotheses h_1 and h_2 on the training set, and $J_D(h_1) < J_D(h_2)$
- If h_2 is "truly" better, i.e. $J^*(h_2) < J^*(h_1)$, our algorithm is overfitting.
- We need theoretical and empirical methods to guard against it!

Typical overfitting plot

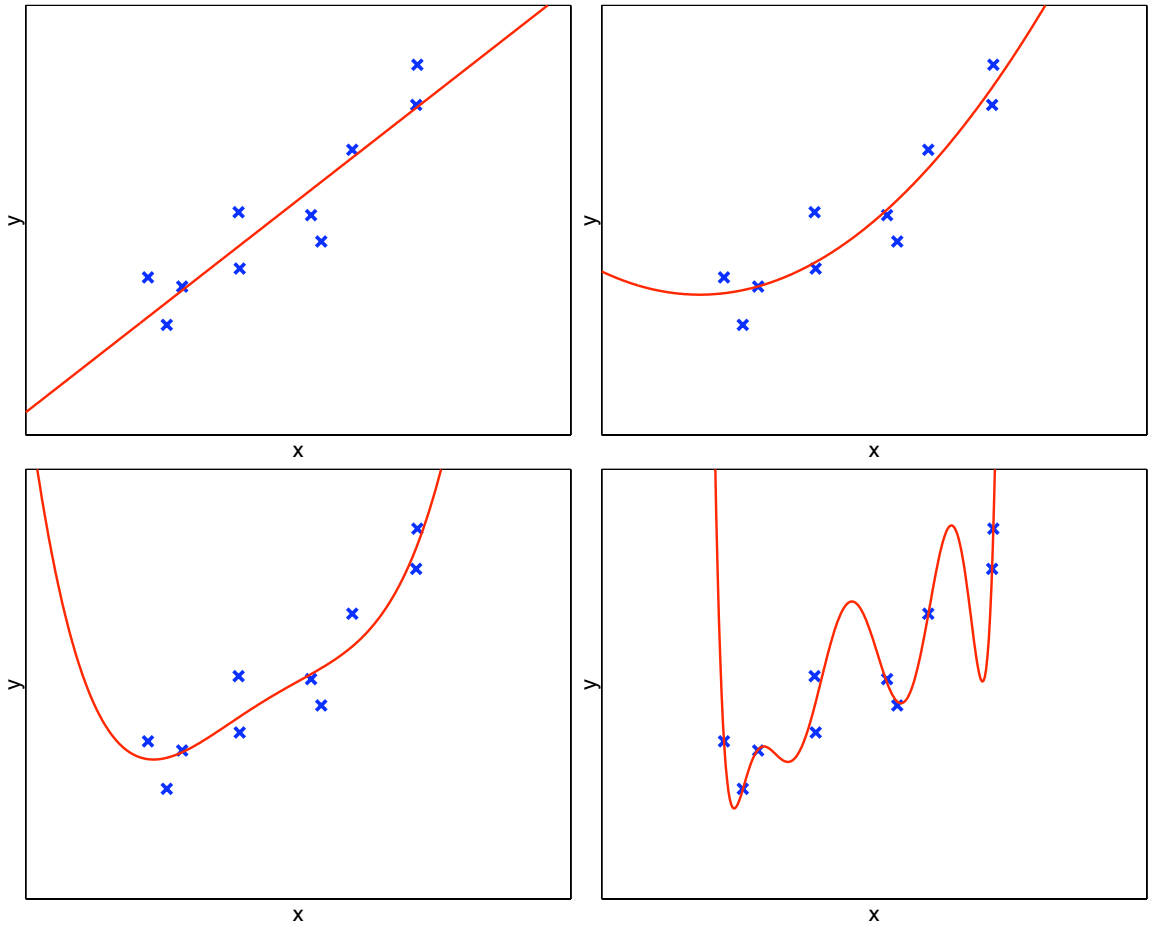


- The training error decreases with the degree of the polynomial M, i.e. *the complexity of the hypothesis*
- The testing error, measured on independent data, decreases at first, then starts increasing
- Cross-validation helps us:
  - Find a good hypothesis class (M in our case), using a *validation set of data*
  - Report unbiased results, using a *test set*, untouched during either parameter training or validation

Cross-validation

- A general procedure for estimating the true error of a predictor
- The available data is split into two subsets:
  - A *training and validation set* used only to find the right predictor
  - A *test set* used to report the prediction error of the algorithm
- These sets *must be disjoint*!
- The process is repeated several times, and the results are averaged to provide error estimates.

Model selection: Polynomial regression



Model selection with leave-one-out cross-validation

1. For each order of polynomial, d:
   (a) Repeat the following procedure m times:
      i. Leave out *ith instance* from the training set, to estimate the true prediction error; we will put it in a *validation set*
      ii. Use all the other instances to find best parameter vector, $\mathbf{w}_{d,i}$
      iii. Measure the error in predicting the label on the instance left out, for the $\mathbf{w}_{d,i}$ parameter vector; call this $J_{d,i}$
      iv. This is a *(mostly) unbiased estimate of the true prediction error*
   (b) Compute the average of the estimated errors: $J_d = \frac{1}{m}\sum_{i=1}^{m} J_{d,i}$
2. Choose the d with lowest average estimated error: $d^* = \arg\min_d J(d)$

Estimating true error for $d = 1$

$D = \{(0.86, 2.49), (0.09, 0.83), (-0.85, -0.25), (0.87, 3.10), (-0.44, 0.87), (-0.43, 0.02), (-1.10, -0.12), (0.40, 1.81), (-0.96, -0.83), (0.17, 0.43)\}$.

Iter	D_{train}	D_{valid}	$\text{Error}_{\text{train}}$	$\text{Error}_{\text{valid}}$ $(J_{1,i})$
1	$D - \{(0.86, 2.49)\}$	$(0.86, 2.49)$	0.4928	0.0044
2	$D - \{(0.08, 0.83)\}$	$(0.09, 0.83)$	0.1995	0.1869
3	$D - \{(-0.85, -0.25)\}$	$(-0.85, -0.25)$	0.3461	0.0053
4	$D - \{(0.87, 3.10)\}$	$(0.87, 3.10)$	0.3887	0.8681
5	$D - \{(-0.44, 0.87)\}$	$(-0.44, 0.87)$	0.2128	0.3439
6	$D - \{(-0.43, 0.02)\}$	$(-0.43, 0.02)$	0.1996	0.1567
7	$D - \{(-1.10, -0.12)\}$	$(-1.10, -0.12)$	0.5707	0.7205
8	$D - \{(0.40, 1.81)\}$	$(0.40, 1.81)$	0.2661	0.0203
9	$D - \{(-0.96, -0.83)\}$	$(-0.96, -0.83)$	0.3604	0.2033
10	$D - \{(0.17, 0.43)\}$	$(0.17, 0.43)$	0.2138	1.0490
		mean:	0.2188	0.3558

Leave-one-out cross-validation results

d	$\text{Error}_{\text{train}}$	$\text{Error}_{\text{valid}}$ (J_d)
1	0.2188	0.3558
2	0.1504	0.3095
3	0.1384	0.4764
4	0.1259	1.1770
5	0.0742	1.2828
6	0.0598	1.3896
7	0.0458	38.819
8	0.0000	6097.5
9	0.0000	6097.5

- Typical overfitting behavior: as d increases, the training error decreases, but the validation error decreases, then starts increasing again
- Optimal choice: $d = 2$. Overfitting for $d > 2$

Estimating both hypothesis class and true error

- Suppose we want to compare polynomial regression with some other algorithm
- We chose the hypothesis class (i.e. the degree of the polynomial, d^*) based on the estimates J_d
- Hence J_{d^*} is *not* unbiased - our procedure was aimed at optimizing it
- If we want to have both a hypothesis class *and* an unbiased error estimate, we need to tweak the leave-one-out procedure a bit

Cross-validation with validation and testing sets

1. For each example j:
   (a) Create a *test set* consisting just of the jth example, $D_j = \{(\mathbf{x}_j, y_j)\}$ and a *training and validation set* $\bar{D}_j = D - \{(\mathbf{x}_j, y_j)\}$
   (b) Use the leave-one-out procedure from above on D_j to find a hypothesis, h_j^*
      - Note that this will split the data internally, in order to both train and validate!
      - Typically, only one such split is used, rather than all possible splits
   (c) Evaluate the error of h_j^* on D_j (call it $J(h_j^*)$)
2. Report the average of the $J(h_j^*)$, as a measure of performance of *the whole algorithm*

Summary of leave-one-out cross-validation

- A very easy to implement algorithm
- Provides a great estimate of the true error of a predictor
- Computational cost scales with the number of instances (examples), so it can be prohibitive, especially if finding the best predictor is expensive
- Alternatives:
  - Leave-k-out generalizes LOO, computationally very expensive.
  - k-fold cross-validation: split the data set into k parts, then proceed as above.

Regularization

- Remember the intuition: complicated hypotheses lead to overfitting
- Idea: change the error function to *penalize hypothesis complexity*:

$$J(\mathbf{w}) = J_D(\mathbf{w}) + \lambda J_{pen}(\mathbf{w})$$

  This is called *regularization* in machine learning and *shrinkage* in statistics
- λ is called *regularization coefficient* and controls how much we value fitting the data well, vs. a simple hypothesis

L_2 regularization for linear models

- *L_2 regularization* (or *weight decay* in neural networks): add a squared penalty on the weights:

$$J_\lambda(\mathbf{w}) = \frac{1}{2}(\mathbf{\Phi w} - \mathbf{y})^\top(\mathbf{\Phi w} - \mathbf{y}) + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

- Why?
  - A simple hypothesis should not be too sensitive to small perturbation of the input
  - Math works out nicely
  - Resolve the issue of $\mathbf{\Phi}^\top\mathbf{\Phi}$ not being invertible in linear regression, e.g. large n small m (original motivation)...

L_2 regularization: closed from solution

$$J_\lambda(\mathbf{w}) = \frac{1}{2}(\mathbf{\Phi w} - \mathbf{y})^\top(\mathbf{\Phi w} - \mathbf{y}) + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

- By re-grouping terms, we get:

$$J_\lambda(\mathbf{w}) = \frac{1}{2}\left(\mathbf{w}^\top(\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathbf{I})\mathbf{w} - \mathbf{w}^\top\mathbf{\Phi}^\top\mathbf{y} - \mathbf{y}^\top\mathbf{\Phi w} + \mathbf{y}^\top\mathbf{y}\right)$$

- Optimal solution (obtained by solving $\nabla J_\lambda(\mathbf{w}) = 0$)

$$\mathbf{w} = (\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathbf{I})^{-1}\mathbf{\Phi}^\top\mathbf{y}$$

(observe that $\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathbf{I}$ is invertible)

Side note: data centering

- For linear regression, we incorporated the bias term in $\mathbf{w} \in \mathbb{R}^{n+1}$ by adding a 1 to each input vector $\mathbf{x} \in \mathbb{R}^n$. Why cannot we do the same for regression with L_2 regularization?
- Instead we center the data, i.e. remove the means from inputs and outputs:
  - Let $\bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^m \mathbf{x}_i$ and $\bar{y} = \frac{1}{m}\sum_{i=1}^m \mathbf{x}_i$.
  - Consider the new data set $\{(\mathbf{x}_i - \bar{\mathbf{x}}, y_i - \bar{y})\}_{i=1}^m$.
  - Solving the regularized regression problem on this new dataset is *equivalent* to solving the original problem
  - You can check that the bias term of the solution on this new data set is 0...

$\hookrightarrow$ exercise

What L_2 regularization does

$$\arg\min_{\mathbf{w}} \frac{1}{2}(\mathbf{\Phi w} - \mathbf{y})^\top(\mathbf{\Phi w} - \mathbf{y}) + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w} = (\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathbf{I})^{-1}\mathbf{\Phi}^\top\mathbf{y}$$

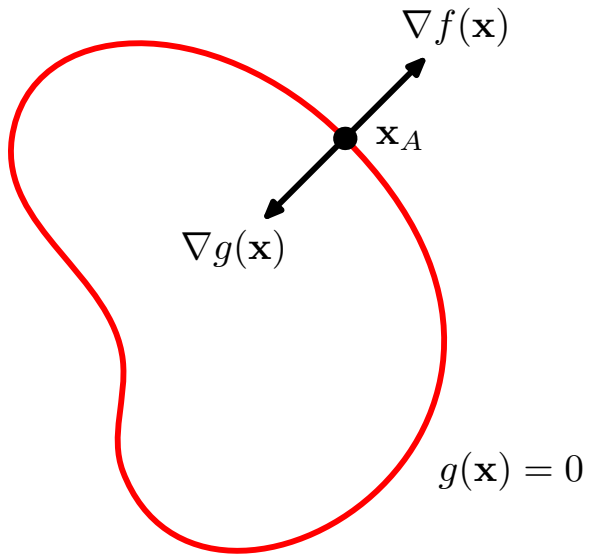
- If $\lambda = 0$, the solution is the same as in regular least-squares linear regression
- If $\lambda \to \infty$, the solution $\mathbf{w} \to 0$
- Positive λ will cause the magnitude of the weights to be smaller than in the usual linear solution
- This is also called *ridge regression*, and it is a special case of Tikhonov regularization (more on that later)
- A different view of regularization: we want to optimize the error while keeping the L_2 norm of the weights, $\mathbf{w}^\top\mathbf{w}$, bounded.

Detour: Constrained optimization

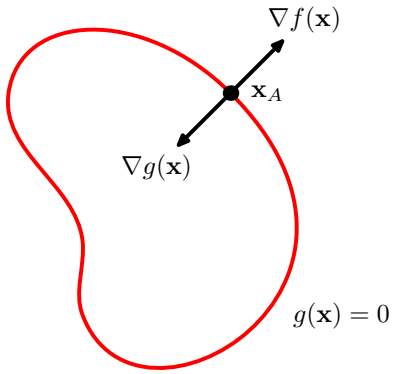
Suppose we want to find

$$\max_{\mathbf{x}} f(\mathbf{x})$$

$$\text{such that } g(\mathbf{x}) = 0$$



Detour: Lagrange multipliers



∇g is orthogonal to the constraint surface (red curve)

- At the optimum:
  - ∇f must be orthogonal to the surface (otherwise we could move along the curve to get a higher value of f)

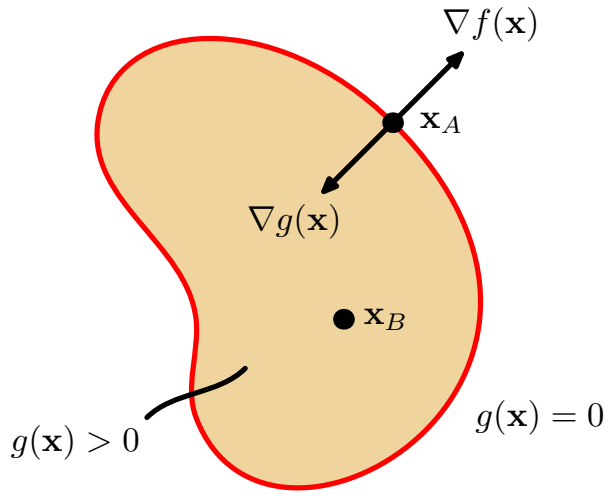
  $\Rightarrow$ ∇f and ∇g have to be parallel

  $\Rightarrow$ There must exist some $\lambda \in \mathbb{R}$ such that $\nabla f + \lambda \nabla g = 0$
- *Lagrangian function*: $L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$ (λ is called *Lagrange multiplier*)
- We obtain the solution to our optimization problem by setting both $\nabla_{\mathbf{x}} L = 0$ and $\frac{\partial L}{\partial \lambda} = 0$

Detour: Inequality constraints

- Suppose we want to find

$$\max_{\mathbf{x}} f(\mathbf{x})$$
$$\text{such that } g(\mathbf{x}) \geq 0$$



- In the interior, $g(\mathbf{x}) > 0$: simply find $\nabla f(\mathbf{x}) = 0$ (in which case $\lambda = 0$ in the Lagrangian)
- On the boundary, $g(\mathbf{x}) = 0$: same situation as before, but the sign matters this time

- For maximization, we want ∇f pointing in the direction opposite to ∇g

Detour: KKT conditions

- Consider again the Lagrangian

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$$

- Based on the previous observations, we minimize L wrt $\mathbf{x}$ subject to the following constraints:

$$\begin{aligned} \lambda &\geq 0 \\ g(\mathbf{x}) &\geq 0 \\ \lambda g(\mathbf{x}) &= 0 \end{aligned}$$

- These are called *Karush-Kuhn-Tucker (KKT) conditions*
- For minimization, simply flip the sign of λ in the Lagrangian:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda g(\mathbf{x})$$

L_2 Regularization for linear models revisited

- Optimization problem: minimize error while keeping norm of the weights bounded

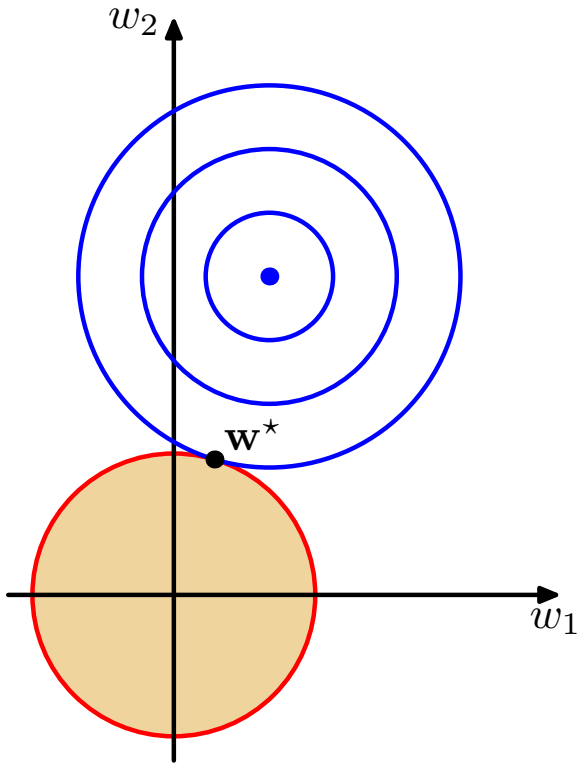
$$\begin{aligned} \min_{\mathbf{w}} J(\mathbf{w}) &= \min_{\mathbf{w}} (\mathbf{\Phi w} - \mathbf{y})^\top (\mathbf{\Phi w} - \mathbf{y}) \\ \text{such that } \mathbf{w}^\top \mathbf{w} &\leq \eta \end{aligned}$$

- The Lagrangian is:

$$L(\mathbf{w}, \nu) = J(\mathbf{w}) - \nu(\eta - \mathbf{w}^\top \mathbf{w})$$

- Fix some λ and let $\mathbf{w}_\lambda$ be the solution of the penalized problem with parameter λ.
- You can check that if $\eta = \|\mathbf{w}_\lambda\|^2$ and $\nu = \lambda$, then $\mathbf{w}_\lambda$ satisfy the KKT conditions, hence the two problems have the same solution.

Visualizing regularization (2 parameters)



$$\mathbf{w}^* = (\mathbf{\Phi}^\top \mathbf{\Phi} + \lambda \mathbf{I})^{-1} \mathbf{\Phi} \mathbf{y}$$

Pros and cons of L_2 regularization

- If λ is at a "good" value, regularization helps to avoid overfitting
- Choosing λ may be hard: cross-validation is often used
- If there are irrelevant features in the input (i.e. features that do not affect the output), L_2 will give them small, but non-zero weights.
- Ideally, irrelevant input should have weights exactly equal to 0.

L_1 Regularization for linear models

- Instead of requiring the L_2 norm of the weight vector to be bounded, make the requirement on the L_1 norm:

$$\begin{aligned} \min_{\mathbf{w}} J_D(\mathbf{w}) &= \min_{\mathbf{w}} (\mathbf{\Phi w} - \mathbf{y})^\top (\mathbf{\Phi w} - \mathbf{y}) \\ \text{such that } \sum_{i=1}^{n} |w_i| &\leq \eta \end{aligned}$$

- This yields an algorithm called Lasso (Tibshirani, 1996)

Solving L_1 regularization

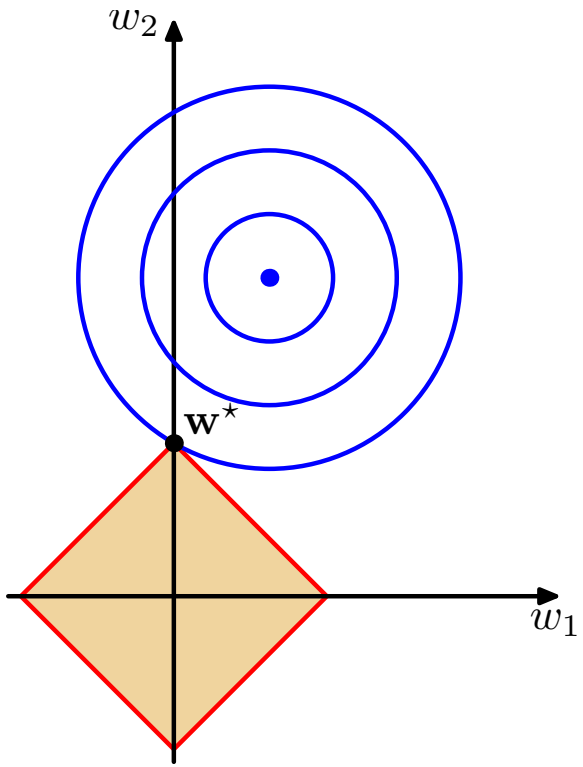
- The optimization problem is a quadratic program
- There is one constraint for each possible sign of the weights (2^n constraints for n weights)
- For example, with two weights:

$$\min_{w_1,w_2} \quad \sum_{j=1}^{m}(y_j - w_1x_1 - w_2x_2)^2$$

$$\begin{aligned} \text{such that } w_1 + w_2 &\leq \eta \\ w_1 - w_2 &\leq \eta \\ -w_1 + w_2 &\leq \eta \\ -w_1 - w_2 &\leq \eta \end{aligned}$$

- Solving this program directly can be done for problems with a small number of inputs

Visualizing L_1 regularization

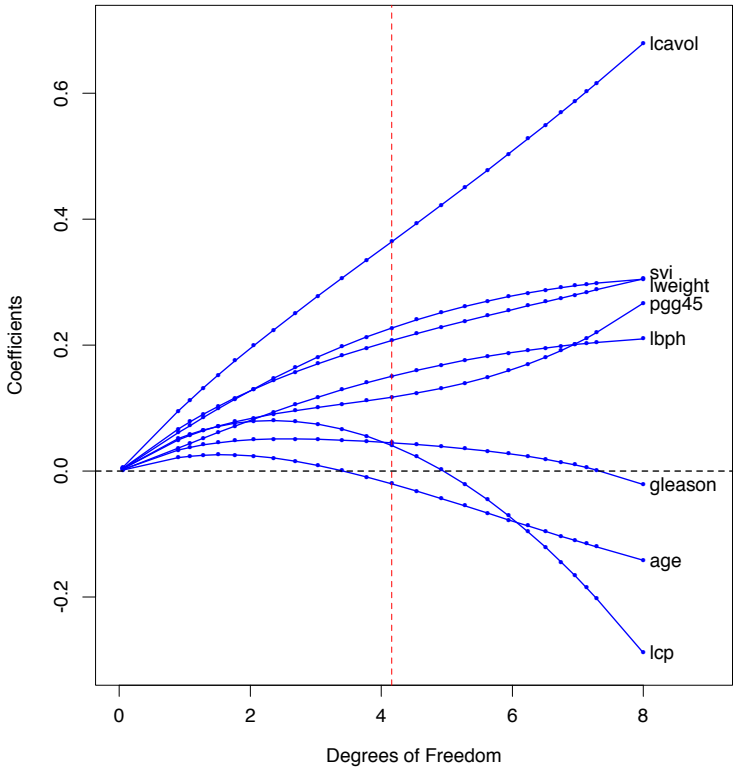


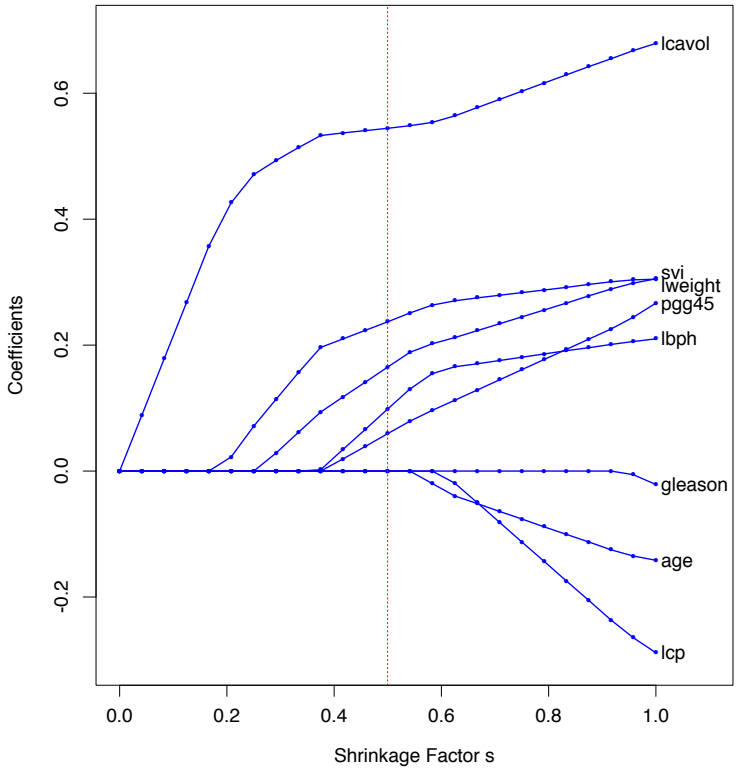
- If λ is big enough, the circle is very likely to intersect the diamond at one of the corners
- This makes L_1 regularization much more likely to make some weights *exactly* 0

Pros and cons of L_1 regularization

- If there are irrelevant input features, Lasso is likely to make their weights 0, while L_2 is likely to just make all weights small
- Lasso is biased towards providing *sparse solutions* in general
- Lasso optimization is computationally more expensive than L_2
- More efficient solution methods have to be used for large numbers of inputs (e.g. least-angle regression, 2003).
- L_1 methods of various types are very popular
- One can combine L_1 and L_2 regularization (elastic-net)

Example of L1 vs L2 effect





- Note the sparsity in the coefficients induces by L_1
- Lasso is an efficient way of performing the L_1 optimization

The anatomy of the error of an estimator

- Suppose we have a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$ where $y = f(\mathbf{x}) + \epsilon$ and ϵ is Gaussian noise with zero mean and standard deviation σ^2
- We fit a linear hypothesis $h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$, such as to minimize sum-squared error over the training data:

$$\sum_{i=1}^{m} (y_i - h(\mathbf{x}_i))^2$$

- Because of the hypothesis class that we chose (hypotheses linear in the parameters) for some target functions f we will have a *systematic prediction error*
- Even if f were truly from the hypothesis class we picked, depending on the data set we have, the parameters $\mathbf{w}$ that we find may be different; this *variability* due to the specific data set on hand is a different source of error

Bias-variance analysis

- Given a new data point $\mathbf{x}$, what is the *expected prediction error*?
- Assume that the data points are drawn *independently and identically distributed (i.i.d.)* from a unique underlying probability distribution $P(\mathbf{x}, y) = P(\mathbf{x})P(y|\mathbf{x})$
- The goal of the analysis is to compute, for an arbitrary given point $\mathbf{x}$,

$$E_P\left[(y - h(\mathbf{x}))^2|\mathbf{x}\right]$$

  where y is the value of $\mathbf{x}$ in a data set, and the expectation is over all training sets of a given size, drawn according to P
- For a given hypothesis class, we can also compute the *true error*, which is the expected error over the input distribution:

$$\sum_{\mathbf{x}} E_P\left[(y - h(\mathbf{x}))^2|\mathbf{x}\right] P(\mathbf{x})$$

  (if $\mathbf{x}$ continuous, sum becomes integral with appropriate conditions).
- We will decompose this expectation into three components

Recall: Statistics 101

- Let X be a random variable with possible values $x_i, i = 1 \ldots n$ and with probability distribution $P(X)$
- The *expected value* or *mean* of X is:

$$E[X] = \sum_{i=1}^{n} x_i P(x_i)$$

- If X is continuous, roughly speaking, the sum is replaced by an integral, and the distribution by a density function
- The *variance* of X is:

$$\begin{aligned} Var[X] &= E[(X - E(X))^2] \\ &= E[X^2] - (E[X])^2 \end{aligned}$$

The variance lemma

$$
\begin{aligned}
Var[X] &= E[(X - E[X])^2] \\
&= \sum_{i=1}^{n} (x_i - E[X])^2 P(x_i) \\
&= \sum_{i=1}^{n} (x_i^2 - 2x_i E[X] + (E[X])^2) P(x_i) \\
&= \sum_{i=1}^{n} x_i^2 P(x_i) - 2E[X] \sum_{i=1}^{n} x_i P(x_i) + (E[X])^2 \sum_{i=1}^{n} P(x_i) \\
&= E[X^2] - 2E[X]E[X] + (E[X])^2 \cdot 1 \\
&= E[X^2] - (E[X])^2
\end{aligned}
$$

We will use the form:

$$E[X^2] = (E[X])^2 + Var[X]$$

Bias-variance decomposition

- Simple algebra:

$$\begin{aligned} E_P\left[(y - h(\mathbf{x}))^2 | \mathbf{x}\right] &= E_P\left[(h(\mathbf{x}))^2 - 2yh(\mathbf{x}) + y^2 | \mathbf{x}\right] \\ &= E_P\left[(h(\mathbf{x}))^2 | \mathbf{x}\right] + E_P\left[y^2 | \mathbf{x}\right] - 2E_P[y|\mathbf{x}]E_P\left[h(\mathbf{x})|\mathbf{x}\right] \end{aligned}$$

- Let $\bar{h}(\mathbf{x}) = E_P[h(\mathbf{x})|\mathbf{x}]$ denote the *mean prediction* of the hypothesis at $\mathbf{x}$, when h is trained with data drawn from P
- For the first term, using the variance lemma, we have:

$$E_P[(h(\mathbf{x}))^2|\mathbf{x}] = E_P[(h(\mathbf{x}) - \bar{h}(\mathbf{x}))^2|\mathbf{x}] + (\bar{h}(\mathbf{x}))^2$$

- Note that $E_P[y|\mathbf{x}] = E_P[f(\mathbf{x}) + \epsilon|\mathbf{x}] = f(\mathbf{x})$ (because of linearity of expectation and the assumption on $\epsilon \sim \mathcal{N}(0, \sigma)$)
- For the second term, using the variance lemma, we have:

$$E[y^2|\mathbf{x}] = E[(y - f(\mathbf{x}))^2|\mathbf{x}] + (f(\mathbf{x}))^2$$

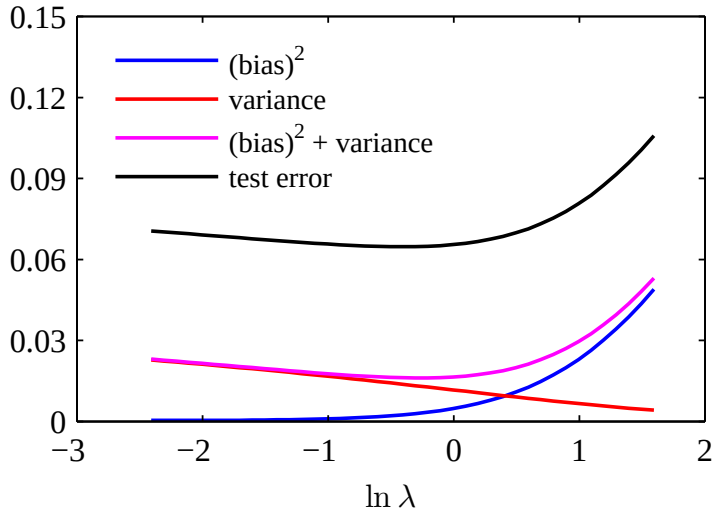
Bias-variance decomposition (2)

- Putting everything together, we have:

$$E_P\left[(y - h(\mathbf{x}))^2|\mathbf{x}\right] = E_P[(h(\mathbf{x}) - \bar{h}(\mathbf{x}))^2|\mathbf{x}] + (\bar{h}(\mathbf{x}))^2 - 2f(\mathbf{x})\bar{h}(\mathbf{x})$$
$$+ E_P[(y - f(\mathbf{x}))^2|\mathbf{x}] + (f(\mathbf{x}))^2$$
$$= E_P[(h(\mathbf{x}) - \bar{h}(\mathbf{x}))^2|\mathbf{x}] \quad + \quad (f(\mathbf{x}) - \bar{h}(\mathbf{x}))^2 \quad + \quad E[(y - f(\mathbf{x}))^2|\mathbf{x}]$$

- The first term, $E_P[(h(\mathbf{x}) - \bar{h}(\mathbf{x}))^2|\mathbf{x}]$, is the *variance* of the hypothesis h at $\mathbf{x}$, when trained with finite data sets sampled randomly from P
- The second term, $(f(\mathbf{x}) - \bar{h}(\mathbf{x}))^2$, is the *squared bias* (or systematic error) which is associated with the class of hypotheses we are considering
- The last term, $E[(y - f(\mathbf{x}))^2|\mathbf{x}]$ is the *noise*, which is due to the problem at hand, and cannot be avoided

Error decomposition



- The bias-variance sum approximates well the test error over a set of 1000 points
- x-axis measures the hypothesis complexity (decreasing left-to-right)
- Simple hypotheses usually have high bias (bias will be high at many points, so it will likely be high for many possible input distributions)
- Complex hypotheses have high variance: the hypothesis is very dependent on the data set on which it was trained.

Bias-variance trade-off

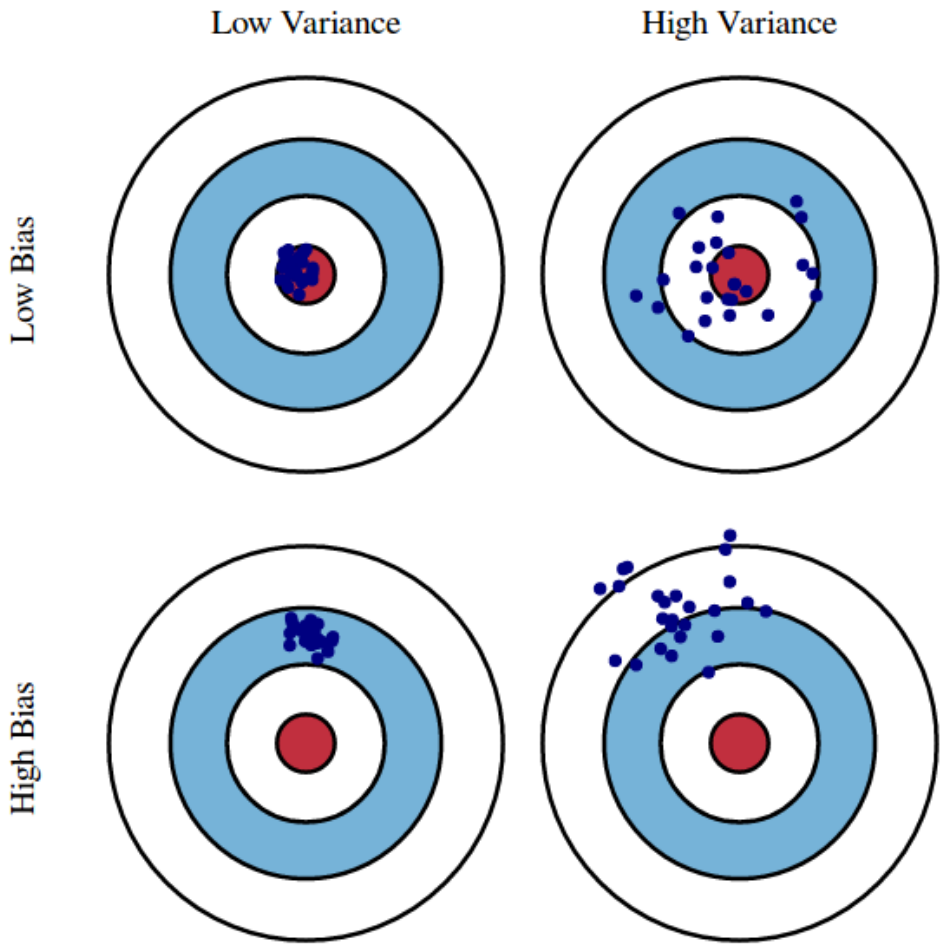


image credit: Scott Fortman-roe (http://scott.fortmann-roe.com/docs/BiasVariance.html)

Bias-variance trade-off

- Typically, bias comes from not having good hypotheses in the considered class
- Variance results from the hypothesis class containing "too many" hypotheses
- MLE estimation is typically unbiased, but has high variance
- Bayesian estimation is biased, but typically has lower variance
- Hence, we are faced with a *trade-off*: choose a more expressive class of hypotheses, which will generate higher variance, or a less expressive class, which will generate higher bias
- Making the trade-off has to depend on the amount of data available to fit the parameters (data usually mitigates the variance problem)

More on overfitting

- Overfitting depends on the amount of data, relative to the complexity of the hypothesis
- With more data, we can explore more complex hypotheses spaces, and still find a good solution