Overfitting regression when the features are noise

We'd like to show that as the number of superfluous features in a regression increases, the variance in the predicted values actually *decreases*.

Setup

Let the labels y be drawn from a normal distribution with mean 1, variance 1: $y \sim N(1,1)$. Similarly let the p-dimensional features x be drawn from a multivariate normal distribution with mean 1 and unit variance: $\mathbf{x} \sim N(\vec{\mathbf{1}}_{1\times p}, I_{p\times p})$. Note that the true model is $h^*(\mathbf{x}) = 1 + \epsilon$, $\epsilon \sim N(0,1)$.

Here we will keep the number of training samples n fixed and vary the number of features. Let Y be the $n \times 1$ response vector and X be the $n \times p$ feature matrix.

Variance of the fitted model

Note 2019-06-11: this derivation isn't what we want, as it is the variance of the test set predictions made by a ridge regression fitted on $X = \mathbf{1}_{n\times p}$

Let $h_{D_n}(\mathbf{x}) = w_1x_1 + w_2x_2 + ... + w_px_p$ be the fitted regression model of a given training set D_n with n examples.

The variance of the predictions over a test set is:

$$\mathrm{Var}[h_{D_n}(\mathbf{x})] = \mathrm{Var}[w_1x_1 + w_2x_2 + ... + w_px_p]$$

Each x_i follows $x_i \sim N(1,1)$, while for a single fitted model the learned w_i's are constant, yielding:

$$\begin{aligned}
\mathrm{Var}[h_{D_n}(\mathbf{x})] &= w_1^2\mathrm{Var}[x_1] + w_2^2\mathrm{Var}[x_2] + ... + w_p^2\mathrm{Var}[x_p] \\
\mathrm{Var}[h_{D_n}(\mathbf{x})] &= \sum_i^p w_i^2
\end{aligned}$$

What we care about however, is the prediction variance of the "average" fitted model $\overline{h}(x)$ on a training set of size n. Following the same algebra as above:

$$\mathrm{Var}[\overline{h}(\mathbf{x})] = \sum_i^p \mathbb{E}[w_i]^2$$

Next, we'll find $\mathbb{E}[w_i]$.

Expected value of the regression coefficients

Our features are Gaussian noise drawn from $N(1,1)$. By "multiplying by one," our feature matrix looks like a $\mathbf{1}_{n\times p}$ matrix with $N(1,1)$ Gaussian noise applied to it: $X = X * \mathbf{1}$. Applying Gaussian noise elementwise to an input matrix is equivalent to applying L2 regularization with regularization parameter $\lambda = n\sigma^2 = n$ [Refs 1, 2].

So, we have a closed form solution for the expected value of the regression coefficients $\mathbf{w}$, where $\mathbf{1}$ is $n \times p$ and I is $p \times p$:

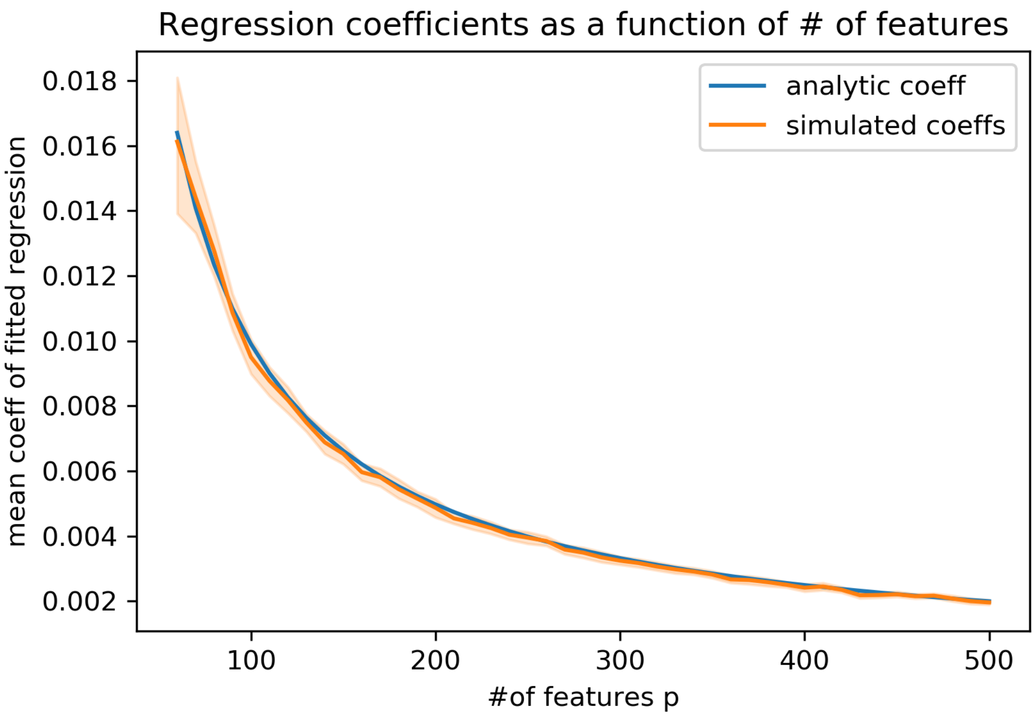
$$\mathbf{w} = (\mathbf{1}^T\mathbf{1} + nI)^{-1}\mathbf{1}^T y$$

The matrix $\mathbf{1}^T\mathbf{1} + nI$ that is being inverted is a $p \times p$ matrix with $2n$ on the main diagonal and n in the off diagonal entries. The inverse of this matrix has $\frac{p}{n(p+1)}$ on the main diagonal and $-\frac{1}{n(p+1)}$ in the off diagonal entries (TODO write up proof).

The expected value of each w_i is then given by:

$$\mathbb{E}[w_i] = \mathbb{E}[\frac{p}{n(p+1)} - (p-1)\frac{1}{n(p+1)}(\sum_i^p y_i)]$$
$$\mathbb{E}[w_i] = \frac{1}{n(p+1)}\mathbb{E}[\sum_i^p y_i]$$
$$\mathbb{E}[w_i] = \frac{1}{n(p+1)}\sum_i^p \mathbb{E}[y_i]$$
$$\mathbb{E}[w_i] = \frac{1}{(p+1)}$$

We verify this via simulation:

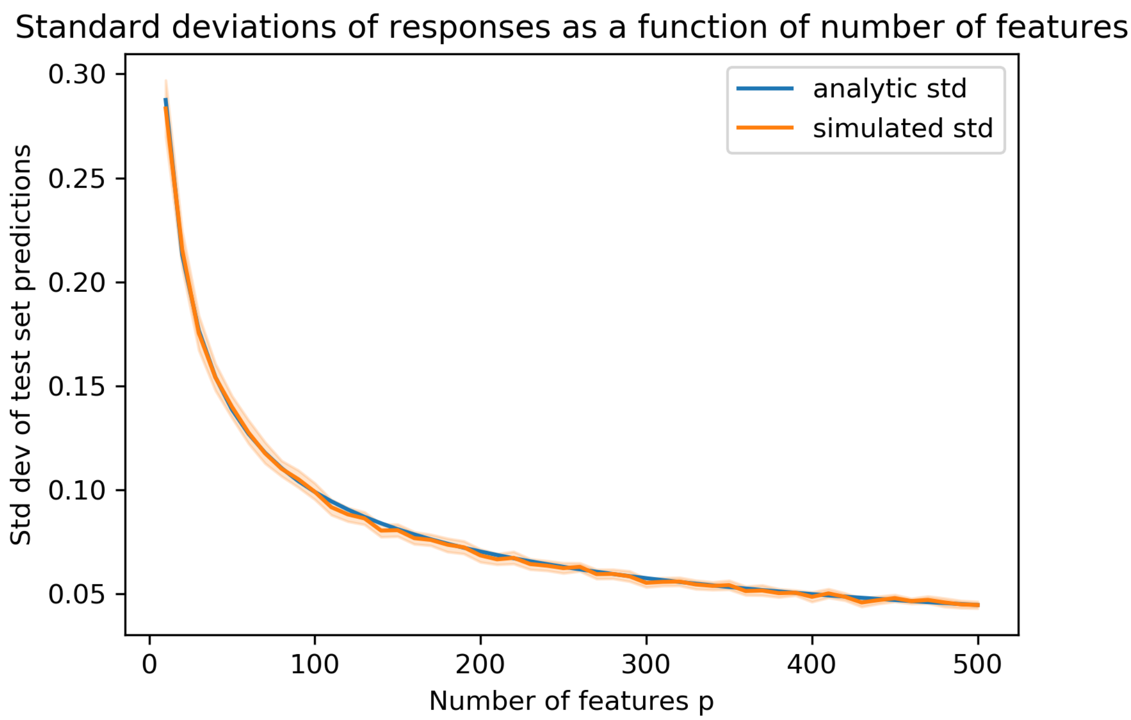


Variance of the fitted model, for fixed constant training data

Using $\mathrm{Var}[\overline{h}(x)] = \sum_i^p \mathbb{E}[w_i^2]$ and $\mathbb{E}[w_i] = \frac{1}{p+1}$, we have that:

$$\mathrm{Var}[\overline{h}(x)] = \frac{p}{(p+1)^2}$$

We see that as the number of uninformative features increases, the variance of the responses of our fitted regression decreases. We verify via simulation:



Contextual note

This is an analogy to overfitting in the general case when adding superfluous features p only contribute noise.