Lecture 7: Regression in Matlab

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Applied Linear Regression in Matlab

```
rng(2017); % set the Random Number Generator
x = linspace(1,15,100)';
y = 2*x + (x+randn(size(x))).^2;
```

Calculating Pseudoinverses

We saw before how the general linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ can be solved for $\boldsymbol{\beta}$ by finding the pseudoinverse $\mathbf{X}^{+}$ of the design matrix $\mathbf{X}$. Then our estimate $\mathbf{b}$ for $\boldsymbol{\beta}$ can be found via matrix multiplication

$$\mathbf{b} = \mathbf{X}^{+}\mathbf{y}$$

For example, given a 5x3 design matrix $\mathbf{X}$

```
X = rand(5,3)
```

```
X =
    0.5978    0.6104    0.7408
    0.8466    0.9087    0.8940
    0.4716    0.8236    0.2554
    0.8076    0.2589    0.9636
    0.5071    0.3713    0.1046
```

and a 5x1 response vector $\mathbf{y}$

```
y = rand(5,1)
```

```
y =
    0.8001
    0.6658
    0.7738
    0.3867
    0.3185
```

we can estimate the parameters $\mathbf{b}$ using the `pinv` function to calculate the pseudoinverse.

```
b = pinv(X)*y
```

```
b =
   -0.0260
    0.8084
    0.1795
```

Matlab also offers the backslash operator (\) to solve linear systems.

```
b = X \ y
```

```
b =
   -0.0260
    0.8084
```

```
0.1795
```

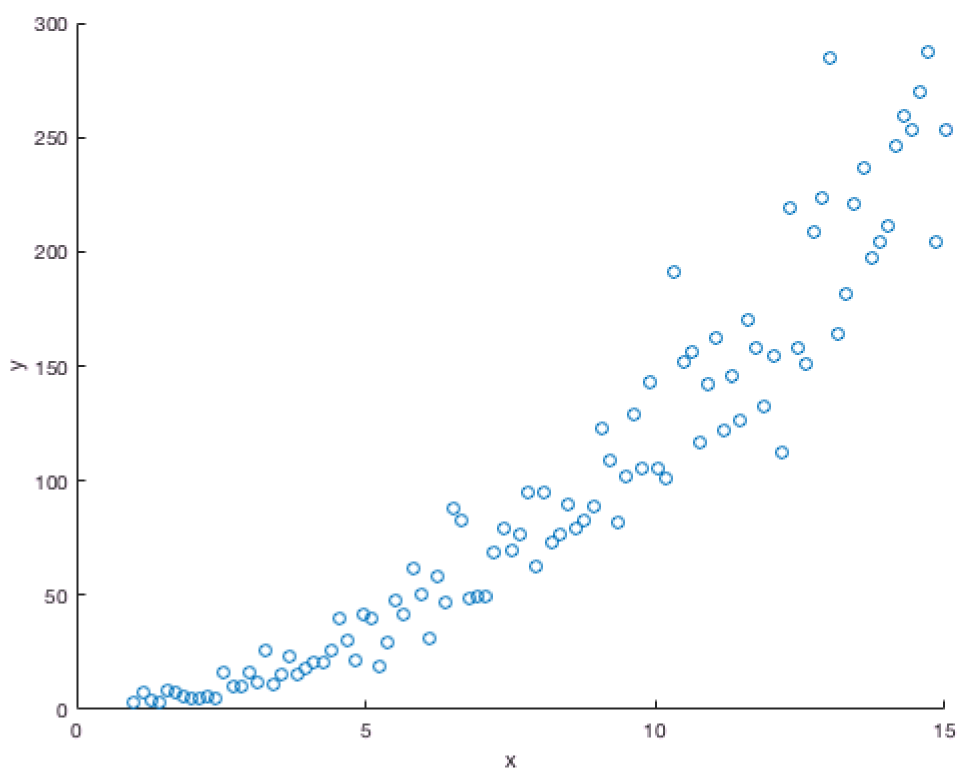
The backslash operator will always choose the appropriate method for solving the system based on the structure of the coefficient matrix. If the coefficient matrix is square and full rank, an efficient variant of Gaussian elimination is selected. If the coefficient matrix is not square, pseudoinversion is used to find the least-squared solution.

Simple Linear Regression

```
rng(2017); % set the Random Number Generator
x = linspace(1,15,100)';
y = 2*x + (x+randn(size(x))).^2;
```

Imagine you are given a set of 100 pairs of data (x, y). We belive that y is some function of x; can we identify this function using linear regression? If possible, we always start by plotting the data. In Matlab, we can use the `scatter` function to visualize individual points.

```
scatter(x,y)
xlabel('x')
ylabel('y')
```



Clearly there is some positive relationship between y and x. Let's begin by fitting the simplest linear model

$$y = \beta_1 x$$

In this case, we only have one parameter to estimate (β_1), and the design matrix $\mathbf{X}$ has only a single column with the 100 x values.

```
X = [x];
```

Let's solve for the parameter estimates by pseudoinversion ($\mathbf{b} = \mathbf{X}^{+}\mathbf{y}$), or, equivalently, using the backslash operator.

```
b = X \ y
```

```
b = 13.3924
```

Let's plot our model on the same plot as the original data. First, we plot the data.

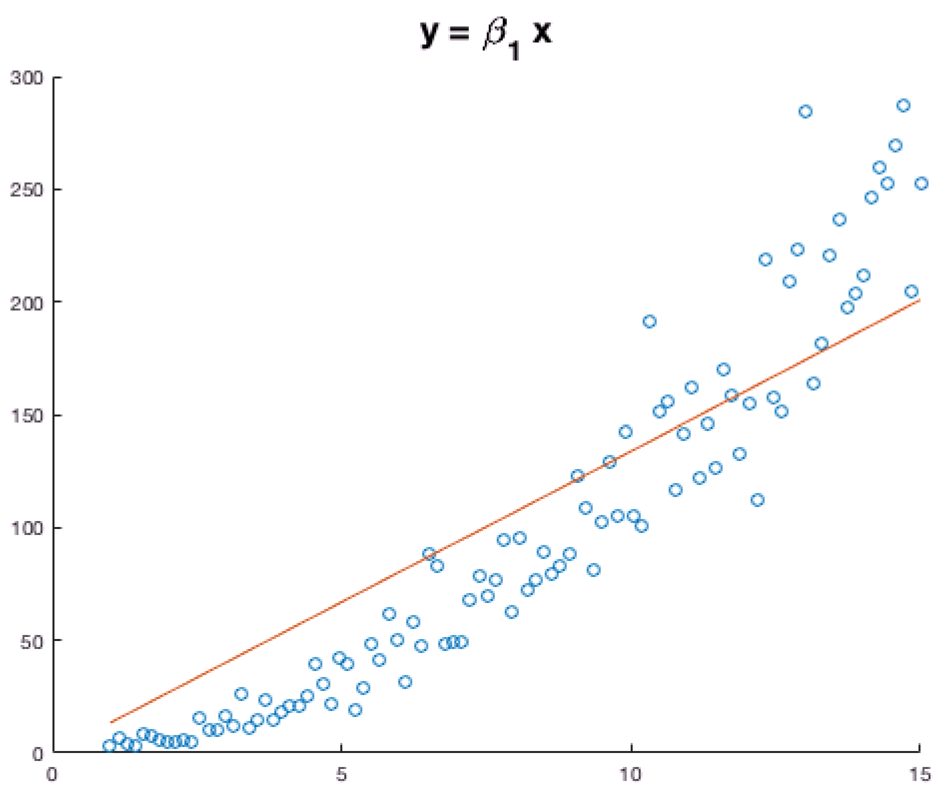
```
scatter(x,y)
```

Then, we tell Matlab to "hold on". This prevents Matlab from making a new figure for subsequent plots (until we tell it to "hold off").

```
hold on
```

Now we can plot a line with our model. The easiest way to multiply the design matrix by the parameter estimates.

```
plot(x, X*b)
title('y = \beta_1 x', 'FontSize',18)
hold off
```



This does not seem to be a great fit. Maybe we need an intercept term, making our model

$$y = \beta_0 + \beta_1 x$$

How do we add an intercept term? We want our final model to be of the form

$$\mathbf{y} = \mathbf{X}\begin{pmatrix}\beta_0 \\ \beta_1\end{pmatrix}$$

This tells us that the design matrix $\mathbf{X}$ should be

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$$

The column of ones on the left allows the parameter β_0 to stand alone as an intercept. Let's construct this design matrix, solve for the parameters, and plot the new model.

```
X = [ones(size(x)) x];
```

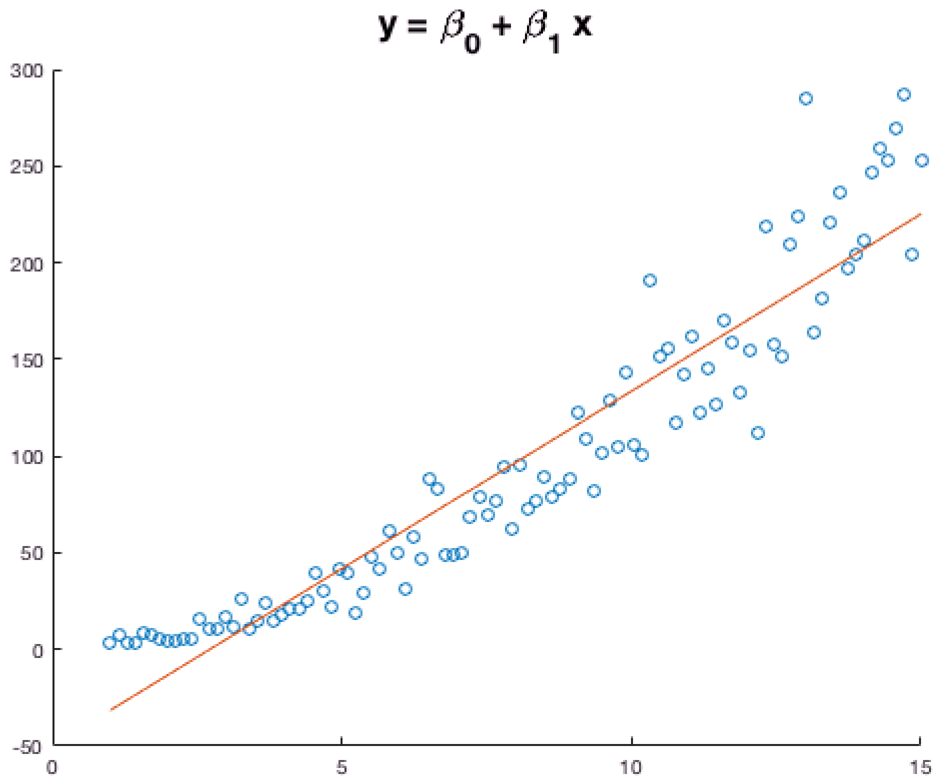
We use the `ones` function to create a column of ones. The `ones` function accepts either two values giving the dimensions (e.g. `ones(3,4)`) or the size of a similar matrix (`ones(size(x))`). Yes, in case you're wondering, there is a `zeros` function.

```
b = X \ y
```

```
b =
  -49.8172
   18.3332
```

The vector b now has two entries. The first is our estimate for β_0, the second is the estimate for β_1.

```
scatter(x,y)
hold on
plot(x, X*b)
title('y = \beta_0 + \beta_1 x', 'FontSize',18)
hold off
```



To plot the line representing our model, we could have constructed the point manually as `b(1) + b(2).*x`. Notice two things. First, Matlab indexes vectors starting at one, so b(1) is actually the estimate for β_0, not for β_1. Second, Matlab distinguishes between matrix multiplication (`*`) and element-by-element multiplication (`.*`).

This is still not a great fit. Based on the slight upward curve in the data, a quadratic model may be more appropriate. This model would be

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

Fortunately, we can still fit quadratic polynomials (and, in fact, all polynomials) since **all polynomials are linear with respect to the parameters**. To fit a quadratic, we add a column to the design matrix that contains the square of each element in the vector x. (We will use the element-by-element exponentiation operator `.^` here; matrix exponentiation is completely different.)

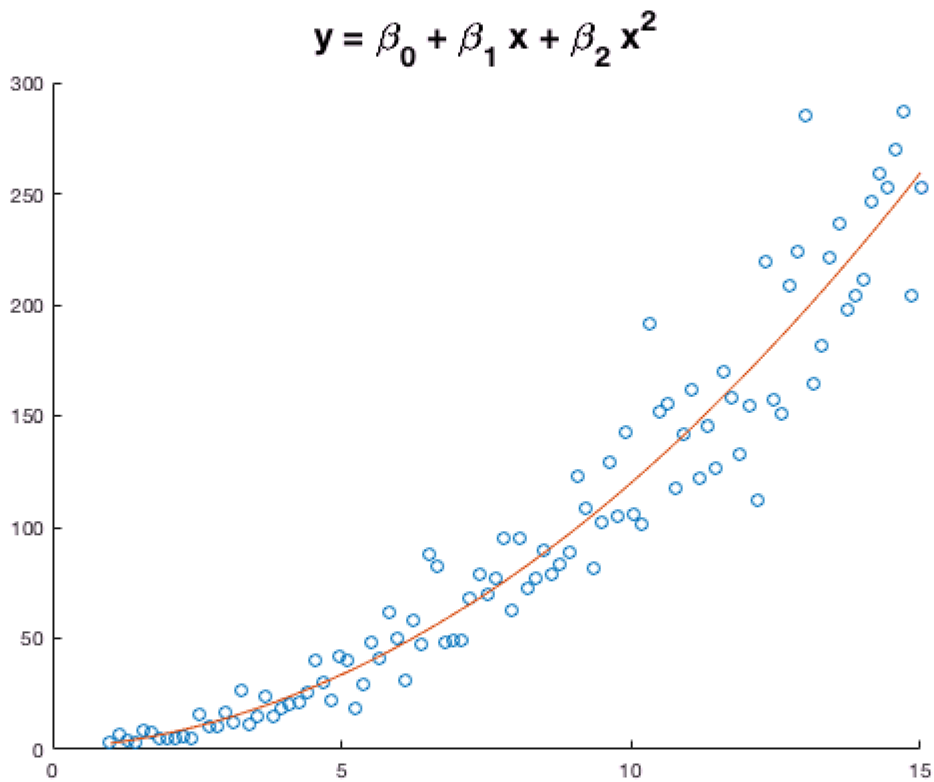
```
X = [ones(size(x))  x  x.^2];
b = X \ y
```

```
b =
    0.3349
    1.3816
    1.0595
```

Our vector of estimates now has three entries corresponding to β_0, β_1, and β_2. Let's plot the quadratic model.

```
scatter(x,y)
hold on
plot(x, X*b)
```

```
title('y = \beta_0 + \beta_1 x + \beta_2 x^2', 'FontSize',18)
hold off
```



That looks like a much better fit. These data appear to have a quadratic relationship.

Linear Regression with `fitlm`

Matlab offers an easier method for fitting linear models -- the `fitlm` function. To use `fitlm`, we start by placing our data in a Matlab table.

```
tbl = table(x,y);
head(tbl) % head shows only a few entries of large tables
```

```
ans = 8×2 table
        x         y
      ______    ______

           1     3.357
      1.1414    7.0774
      1.2828    3.6488
      1.4242    2.8731
      1.5657    8.2716
      1.7071    7.6963
      1.8485    5.3921
      1.9899    4.6634
```

Each variable given to the `table` function becomes a column in the table. The names of the columns are the names of the variables in the call to `table`. (If Matlab can't find the names, for example if you call `table(log(x), y+3)`, it names the columns "Var1", "Var2", etc.). You can change the names of an existing table by setting `tbl.Properties.VariableNames = {'name1', 'name2', ...}`.

The column names are important, as we refer to variables by these names when specifying our linear model.

Now that we have our data in a table, we call `fitlm`.

```
model1 = fitlm(tbl, 'y ~ x')
```

```
model1 =

Linear regression model:
    y ~ 1 + x

Estimated Coefficients:
                   Estimate      SE        tStat       pValue
                   ________    _______    _______    __________

    (Intercept)    -49.817      5.7739    -8.6281    1.1389e-13
    x               18.333     0.64288     28.517    3.0026e-49


Number of observations: 100, Error degrees of freedom: 98
Root Mean Squared Error: 26.2
R-squared: 0.892,  Adjusted R-Squared 0.891
F-statistic vs. constant model: 813, p-value = 3e-49
```

The first argument to `fitlm` is the table containing your data. The second argument is a string specifying the formula for the linear model. To specify a formula:

- Use a tilde to separate the response variable (y) from the input variables (x_1, x_2, etc.).
- Do not include the names of the parameters; only the input variables. For example, we say `'y ~ x'` not `'y ~ b*x'`. The `fitlm` function adds a parameter for each term in the model.
- `fitlm` always adds an intercept by default. To turn off this behavior, call `fitlm` with the `'intercept'` option set to false, i.e. `fitlm(..., 'intercept', false)`.
- The names of the response and input variables must match column names in the table.

The output from `fitlm` begins by stating the specified model. Again, no parameters appear. If an intercept was added, it appears as a 1 (just like the column of ones in the design matrix). Next is a table of the fit parameters -- an estimate of each coefficient in the model, including the intercept. Along with providing the numerical value of the coefficient, `fitlm` also reports the standard error for the estimate. The standard errors are calculated using the degrees of freedom left over in the data. So long as the number of observations is greater than the number of variables, `fitlm` will be able to provide errors for each coefficient.

Using the standard errors, we can construct confidence intervals around the parameter estimates. It is important to know if the confidence interval includes zero. If so, then we cannot reject the possibility that the true value of the parameter is zero. If the true value is zero, we should not draw any inferences regarding the estimated coefficient, since we cannot statistically distinguish the parameter from zero. To help identify statistically significant parameters, `fitlm` performs a modified *t*-test on the parameter estimates. Using the *t*-statistic ("tStat" in the `fitlm` output), a *p*-value is calculated. Only those estimates with *p*-values below out significance threshold (e.g. 0.05) should be interpreted.

`fitlm` also provides summary statistics on the model as a whole. The most commonly used metris is the coefficient of determination (R^2). Values near one are ideal; however, there is not widely accepted cutoff for "good" vs. "bad" R^2 values. Instead, you should consider the *F*-statistic. This test measures if the model performs better than a null model -- a model that discards the inputs and returns only a constant value.

Finally, `fitlm` provides the root mean squared error (RMSE). This measures the accuracy of the model and summarizes how closely estimates made with the model match the observed responses. To calculate the RMSE, we use the observed responses (y_i) and the predicted responses ($\hat{y}_i$) from our model on the corresponing inputs (x_i). Then the RMSE is

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2}$$

The RMSE is the square root of the average penalty (the squared error) found during the least squares estimation.

Let's use `fitlm` to fit our quadratic model.

```
model2 = fitlm(tbl, 'y ~ x^2')
```

```
model2 = 

Linear regression model:
    y ~ 1 + x + x^2

Estimated Coefficients:
                   Estimate      SE        tStat        pValue  
                   ________    _______    ________    __________

    (Intercept)    0.33485      8.0944    0.041369       0.96709
    x               1.3816      2.3069     0.59887       0.55065
    x^2             1.0595     0.14057       7.537    2.5514e-11


Number of observations: 100, Error degrees of freedom: 97
Root Mean Squared Error: 20.9
R-squared: 0.932,  Adjusted R-Squared 0.931
F-statistic vs. constant model: 667, p-value = 2.1e-57
```

For convenience, adding a quadratic term in the `fitlm` formula expands to include the linear term. This behavior can be disabled using the `'purequadratic'` option.

Exploratory Data Analysis with Linear Models

We can use linear modeling to identify factors that significantly affect an outcome. For example, lets use Matlab's builtin set of simulated hospital records.

```
load hospital_records
hospital(1:10,:)
```

```
ans = 
               LastName          Sex       Age    Weight    Smoker    BloodPressure
    YPL-320    'SMITH'           Male      38     176       true      124           93
    GLI-532    'JOHNSON'         Male      43     163       false     109           77
    PNI-258    'WILLIAMS'        Female    38     131       false     125           83
    MIJ-579    'JONES'           Female    40     133       false     117           75
    XLK-030    'BROWN'           Female    49     119       false     122           80
    TFP-518    'DAVIS'           Female    46     142       false     121           70
    LPD-746    'MILLER'          Female    33     142       true      130           88
    ATA-945    'WILSON'          Male      40     180       false     115           82
    VNL-702    'MOORE'           Male      28     183       false     115           78
    LQW-768    'TAYLOR'          Female    31     132       false     118           86
```

We want to identify any factors (sex, age, weight, or smoking) that increase blood pressure. We will build a linear model that combines these factors to predict blood pressure. First, let's average the systolic and diastolic blood pressures into a single value that we can use as our response variable.

```
hospital.meanBP = mean(hospital.BloodPressure,2);
hospital(1:10,:)
```

```
ans =
              LastName          Sex       Age    Weight    Smoker    BloodPressure      meanBP
    YPL-320   'SMITH'           Male      38     176       true      124          93    108.5
    GLI-532   'JOHNSON'         Male      43     163       false     109          77       93
    PNI-258   'WILLIAMS'        Female    38     131       false     125          83      104
    MIJ-579   'JONES'           Female    40     133       false     117          75       96
    XLK-030   'BROWN'           Female    49     119       false     122          80      101
    TFP-518   'DAVIS'           Female    46     142       false     121          70     95.5
    LPD-746   'MILLER'          Female    33     142       true      130          88      109
    ATA-945   'WILSON'          Male      40     180       false     115          82     98.5
    VNL-702   'MOORE'           Male      28     183       false     115          78     96.5
    LQW-768   'TAYLOR'          Female    31     132       false     118          86      102
```

We added another column, "meanBP" to the `hospital` table. The second argument to mean tells the function to calculate the means along the second dimension. This gives us the mean for each row.

Now we build and fit a linear model using fitlm.

```
fitlm(hospital, 'meanBP ~ Sex + Age + Weight + Smoker')
```

```
ans =

Linear regression model:
    meanBP ~ 1 + Sex + Age + Weight + Smoker

Estimated Coefficients:
                   Estimate        SE         tStat        pValue
                  __________    ________    _________    __________

    (Intercept)        97.09      5.4093       17.949    2.7832e-32
    Sex_Male         0.51095      2.0897      0.24451       0.80737
    Age             0.058337    0.047726       1.2224        0.2246
    Weight        -0.0008026    0.039503    -0.020317       0.98383
    Smoker_1          10.088     0.73786       13.672    3.6239e-24


Number of observations: 100, Error degrees of freedom: 95
Root Mean Squared Error: 3.41
R-squared: 0.683,  Adjusted R-Squared 0.67
F-statistic vs. constant model: 51.2, p-value = 6.55e-23
```

Looking at the coefficient estimates, we find that only smoking is a significant predictor. The coefficient is 10.1, so smokers on average have a blood pressure that is 10 mmHg higher than non-smokers.

Be careful in interpreting the intercept of this model. The intercept is the response value when all inputs are zero. For this example, all zero inputs would be a female non-smoker of age zero that weighs nothing. Instead, we can find an average blood pressure for a 30 year old, 100 pound female nonsmoker as

$$\mathrm{BP} = 97.1 + 0.51(0) + 0.058(30) - 0.00080(100) + 10.1(0) = 98.8$$

For a 50 year old, 260 pound male smoker, the estimate would be

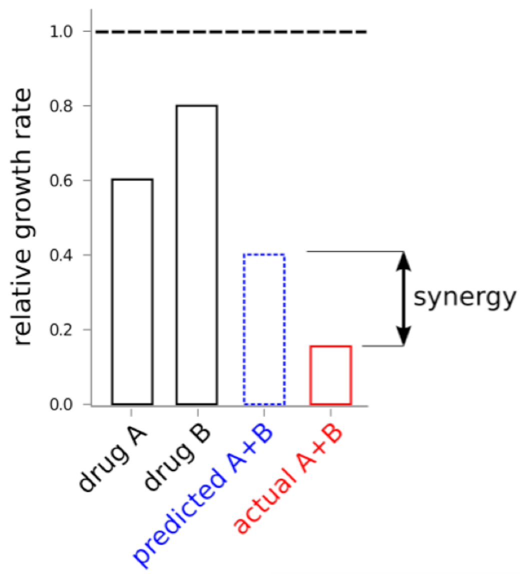
$$BP = 97.1 + 0.51(1) + 0.058(50) - 0.00080(260) + 10.1(1) = 110.4$$

Interactions

```
rng(61112);

conc_A = rand(15,1);
conc_B = rand(15,1);
response = 3.*conc_A + 4.5.*conc_B + 12.5.*conc_A.*conc_B + 0.5.*randn(15,1);
drug = table(response, conc_A, conc_B);
```

Linear models can test for significant interactions between variables. To include interactions between variables x_i and x_j, we add a new term that is the product of the two variables ($x_i x_j$). We choose multiplication to combine the variables since this interaction term will only be nonzero when **both** variables are nonzero; thus, the interaction is suppressed when either variable is not observed.

Interactions are commonly used to test for *synergy* between drugs. For drugs to synergize, the observed response must be greater than the expected additive effects of the two drugs alone. (If the drugs response is lower than expected, the drugs are *antagonistic*.)



We modeled the response to the drug (y) as a linear combination of the two drugs independently plus an interaction term:

$$y = \beta_0 + \beta_1[c_1] + \beta_2[c_2] + \beta_{12}[c_1][c_2]$$

where $[c_1]$ is the concentration of drug 1 (or log-concentration, as dose responses are often log-linear), and $[c_2]$ is the concentration of drug 2. The intercept (β_0) is the basal response of the assay when neither drug is added. The parameter β_{12} corresponds to the strength of the interaction. If we fit the above model and find a significant, nonzero β_{12} term, we can conclude that some nonlinear interaction exists between the drugs.

Let's test for synergy with the following drug response data (with concentration is log scale).

```
drug
```

drug = *15×3 table*

```
response     conc_A      conc_B
________    ________    ________

2.9375       0.78812    0.056482
6.9199       0.48957     0.51783
2.6542       0.53637    0.075296
9.3316       0.32535     0.88539
 8.567       0.82917     0.34905
16.306       0.98211     0.80744
1.6428       0.63671    0.017543
5.6819      0.070839     0.93119
2.5009       0.54116    0.079158
3.9707       0.89685    0.029386
2.2057       0.62384    0.043192
 13.62       0.60518     0.98991
14.015         0.892     0.74739
 4.924       0.37901     0.39126
 4.993       0.15946      0.6222
```

In `fitlm` formulas, interactions are specified by combining the two variable names with a colon (`x1:x2`). As a shortcut, we can add both linear terms and an interaction term using the * operator. The formula `response ~ x1 + x2 + x1:x2` is equivalent to the formula `response ~ x1 * x2`.

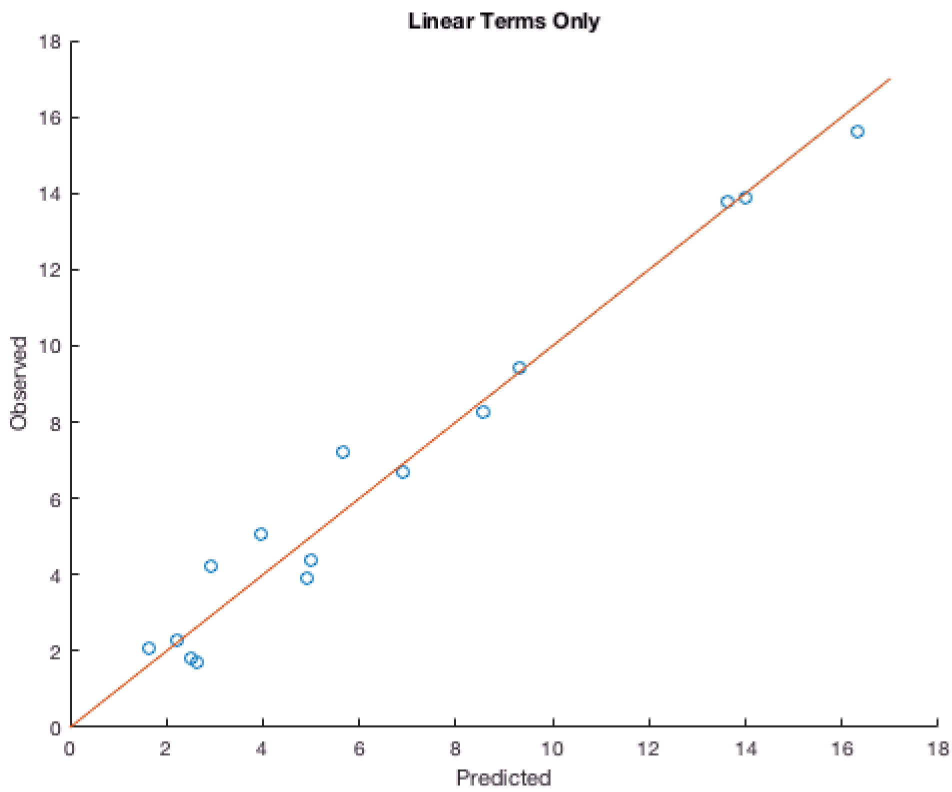
First, let's fit a linear model without interaction.

```
model_lin = fitlm(drug, 'response ~ conc_A + conc_B')
```

```
model_lin = 

Linear regression model:
    response ~ 1 + conc_A + conc_B

Estimated Coefficients:
                   Estimate      SE        tStat       pValue  
                   ________    _______    _______    __________

    (Intercept)    -5.0689     0.69951    -7.2464    1.0197e-05
    conc_A          10.887     0.89216     12.202    4.0126e-08
    conc_B          12.378     0.64862     19.083    2.4105e-10


Number of observations: 15, Error degrees of freedom: 12
Root Mean Squared Error: 0.861
R-squared: 0.972,  Adjusted R-Squared 0.967
F-statistic vs. constant model: 205, p-value = 5.28e-10
```

We would like to plot the data and our model. Unfortunately, the multiple input variables makes visualization difficult. Instead, we can get a sense for our model's accuracy by plotting the observed response values vs. the model's predicted response values. (We use the predict function to find the predicted values from a fitted model and the original data table. We also add a diagonal line corresponding to perfect correlation.)

```
scatter(drug.response, predict(model_lin,drug))
xlabel('Predicted');
ylabel('Observed');
title('Linear Terms Only');
hold on
plot([0 17], [0 17])
hold off
```



This isn't a bad model fit, but it can clearly be improved. Maybe the interaction terms will help.

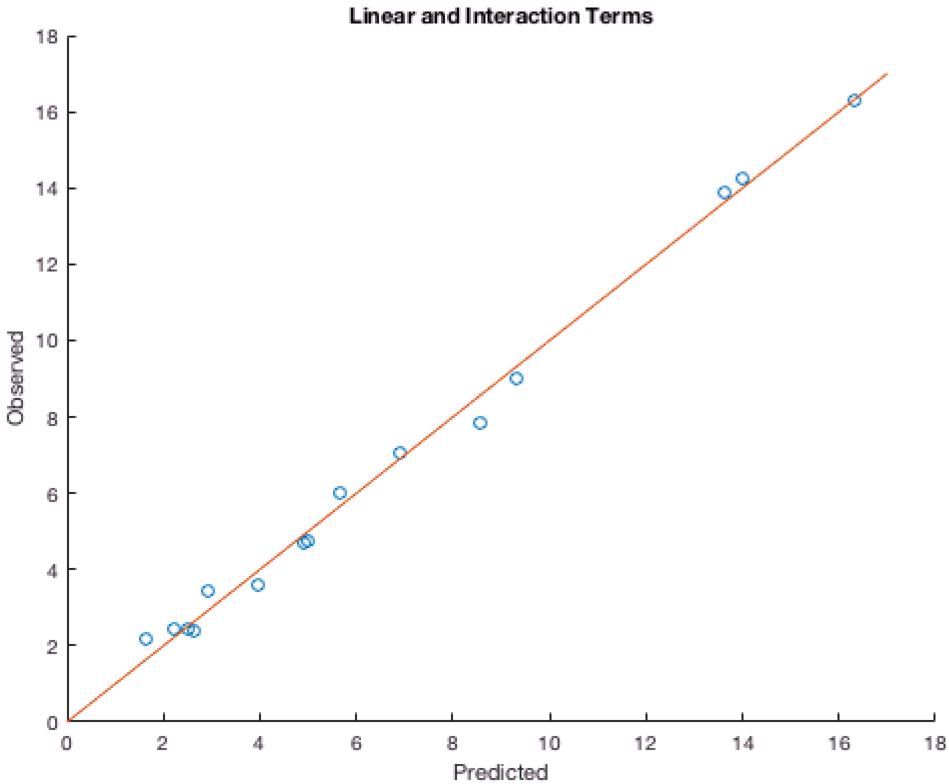
```
model_int = fitlm(drug, 'response ~ conc_A * conc_B')
```

```
model_int = 

Linear regression model:
    response ~ 1 + conc_A*conc_B

Estimated Coefficients:
                     Estimate       SE        tStat       pValue  
                     ________    _______     ______    __________

    (Intercept)      -0.94009    0.71872     -1.308       0.21755
    conc_A             4.5727     1.0626     4.3034     0.0012489
    conc_B               6.44    0.96668      6.662    3.5531e-05
    conc_A:conc_B      9.4829     1.4631     6.4815    4.5414e-05


Number of observations: 15, Error degrees of freedom: 11
Root Mean Squared Error: 0.409
R-squared: 0.994,  Adjusted R-Squared 0.992
F-statistic vs. constant model: 618, p-value = 1.55e-12
```

The coefficient of the interaction term is statistically significant at $p < 0.05$. The coefficient is also positive, indicating synergy between the drugs. Let's see if taking the synergy into account improves our predictions.

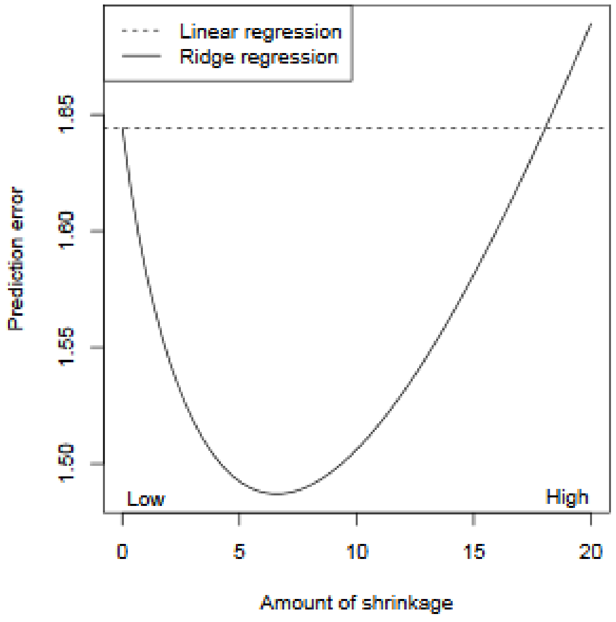
```
scatter(drug.response, predict(model_int,drug))
xlabel('Predicted');
ylabel('Observed');
```

```
title('Linear and Interaction Terms');
hold on
plot([0 17], [0 17])
hold off
```



The model with the interaction term is a better predictor of the drug response.

Regularization



Shrinks the magnitude of coefficients

Bias: error from erroneous assumptions about the training data

- High bias (underfitting) → miss relevant relations between predictors & target

Variance: error from sensitivity to small fluctuations in the training data

- High variance (overfitting) → model random noise and not the intended output

Bias – variance tradeoff: Ignore some small details, to get a more general "big picture"

Ridge regression

Given a vector with observations $y \in \mathbb{R}^n$ and a predictor matrix $X \in \mathbb{R}^{n \times p}$

the ridge regression coefficients are defined as:

$$\begin{aligned}\hat{\beta}^{\text{ridge}} &= \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \\ &= \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \underbrace{\|y - X\beta\|_2^2}_{\text{Loss}} + \lambda \underbrace{\|\beta\|_2^2}_{\text{Penalty}}\end{aligned}$$

Not only minimizing the squared error, but also the size of the coefficients!

Ridge regression

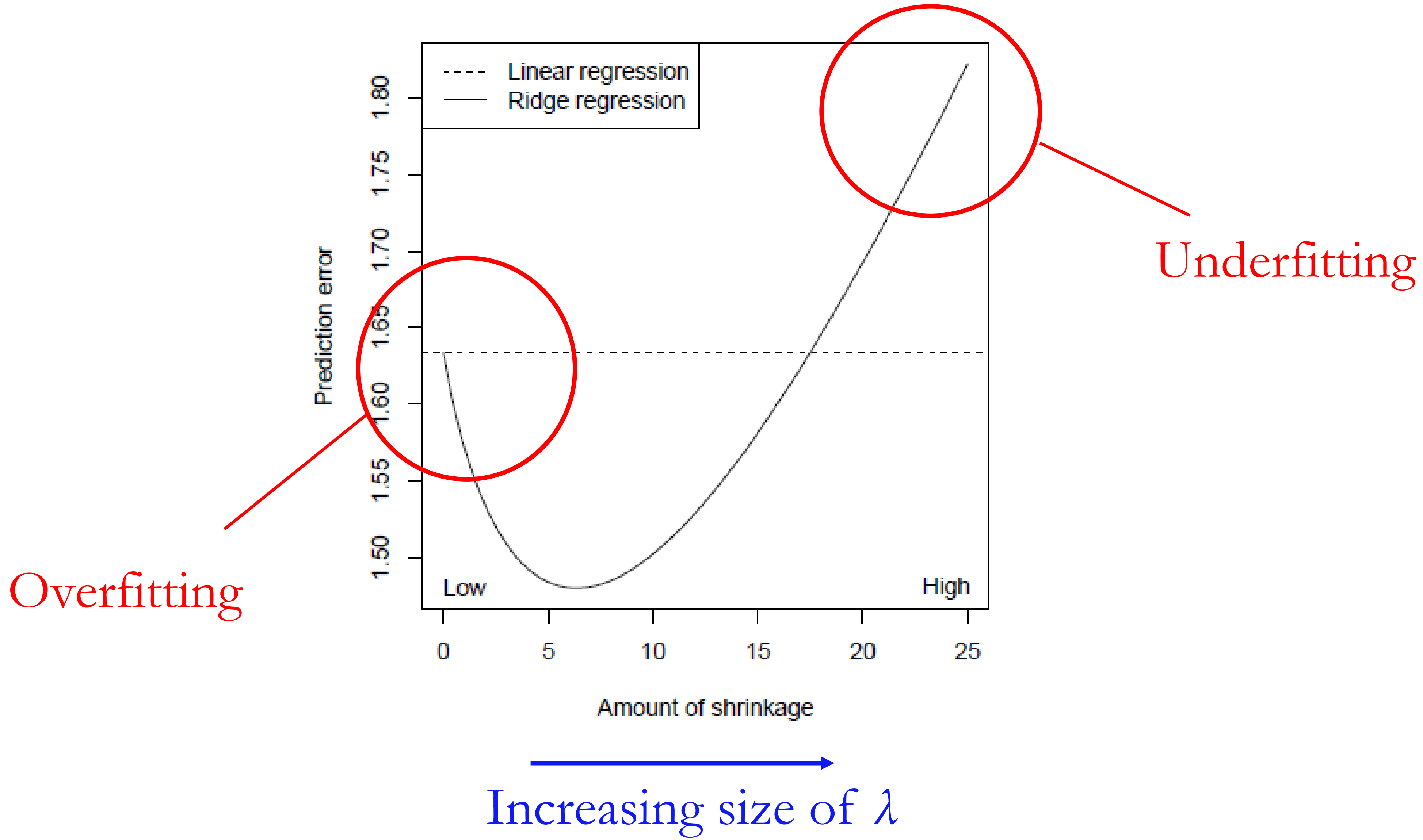
Here, $\lambda \geq 0$ is a tuning parameter for controlling the strength of the penalty

- When $\lambda = 0$, we minimize only the loss → overfitting
- When $\lambda = \infty$, we get $\hat{\beta}^{\text{ridge}} = 0$ that minimizes the penalty → underfitting

When including an intercept term, we usually leave this coefficient unpenalized

$$\hat{\beta}_0, \hat{\beta}^{\text{ridge}} = \underset{\beta_0 \in \mathbb{R},\, \beta \in \mathbb{R}^p}{\operatorname{argmin}} \ \|y - \beta_0 \mathbb{1} - X\beta\|_2^2 + \lambda \|\beta\|_2^2$$

Example 3



Linear regression
Ridge regression
Prediction error
1.80
1.75
1.70
1.65
1.60
1.55
1.50
Low
High
0
5
10
15
20
25
Amount of shrinkage
Overfitting
Underfitting
Increasing size of λ

Variable selection

Problem of selecting the most relevant predictors from a larger set of predictors

In linear model setting, this means estimating some coefficients to be exactly zero

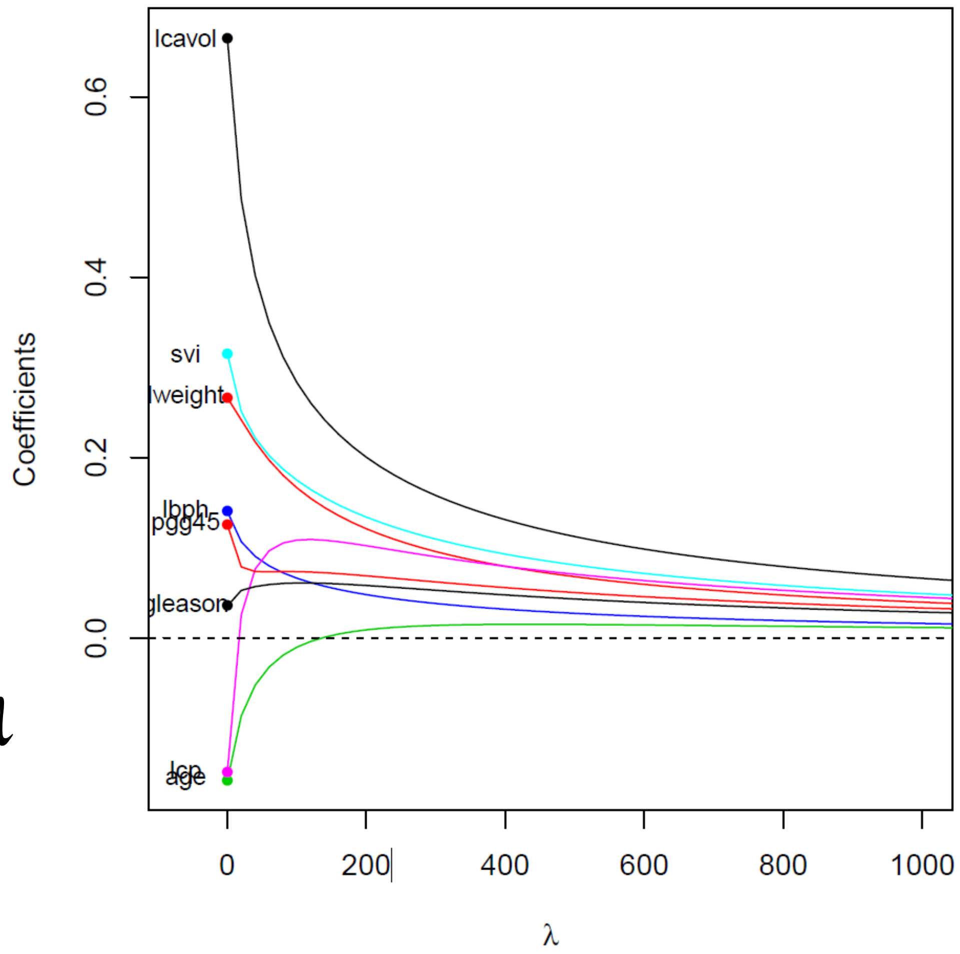
This can be very important for the purposes of model interpretation

Ridge regression cannot perform variable selection

- Does not set coefficients exactly to zero, unless $\lambda = \infty$

Example 4

Suppose that we are studying the level of prostate-specific antigen (PSA), which is often elevated in men who have prostate cancer. We look at n = 97 men with prostate cancer, and p = 8 clinical measurements. We are interested in identifying a small number of predictors, say 2 or 3, that drive PSA.



We perform ridge regression over a wide range of λ

This does not give us a clear answer...

Solution: Lasso regression

Lasso regression

The lasso coefficients are defined as:

$$\hat{\beta}^{\text{lasso}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \|y - X\beta\|_2^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$= \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \underbrace{\|y - X\beta\|_2^2}_{\text{Loss}} + \lambda \underbrace{\|\beta\|_1}_{\text{Penalty}}$$

The only difference between lasso & ridge regression is the penalty term

- Ridge uses ℓ_2 penalty $\|\beta\|_2^2$
- Lasso uses ℓ_1 penalty $\|\beta\|_1$

Lasso regression

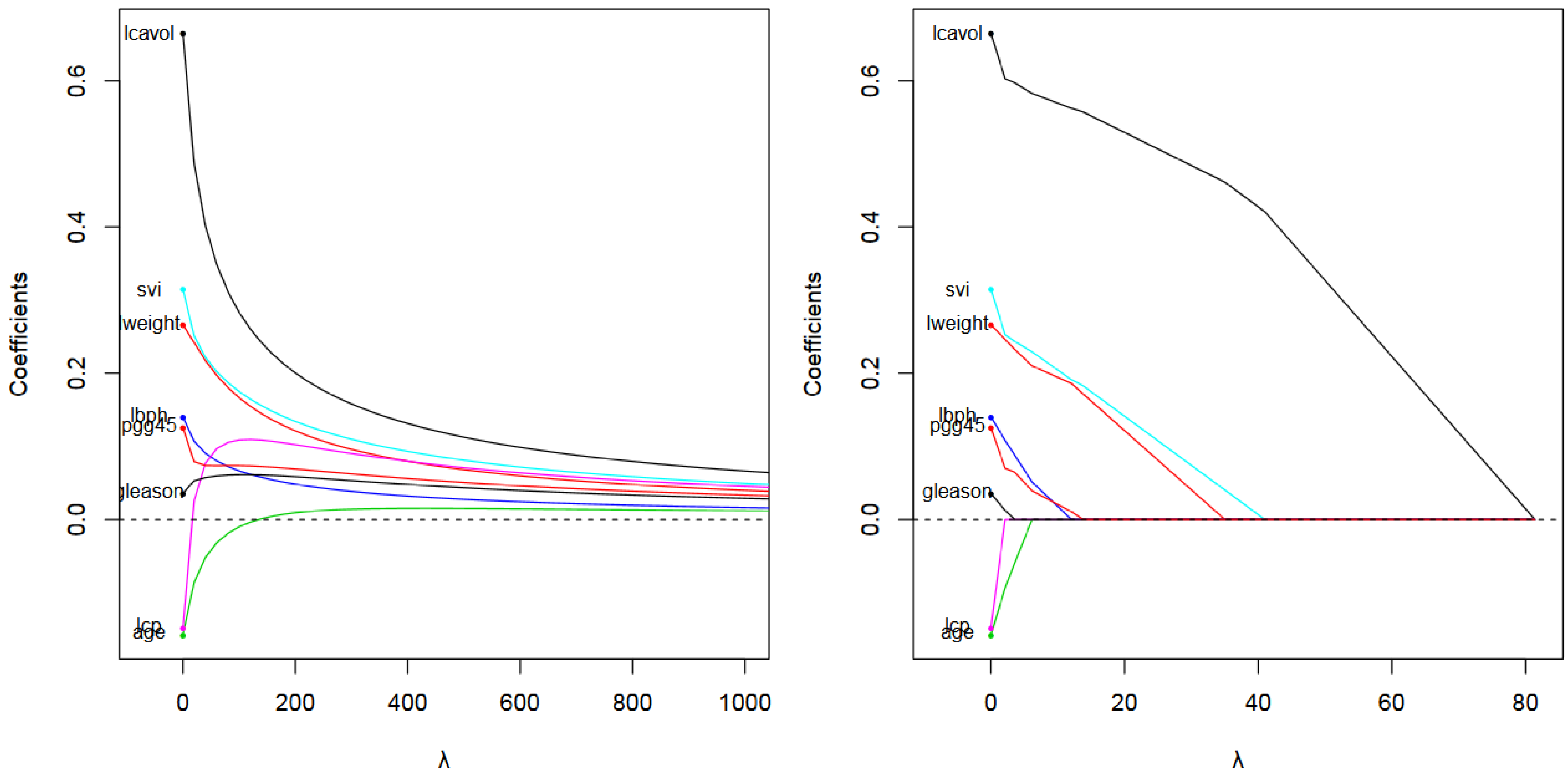
Again, λ ≥ 0 is a tuning parameter for controlling the strength of the penalty

The nature of the l_1 penalty causes some coefficients to be shrunken to zero exactly

As λ increases, more coefficients are set to zero → less predictors are selected

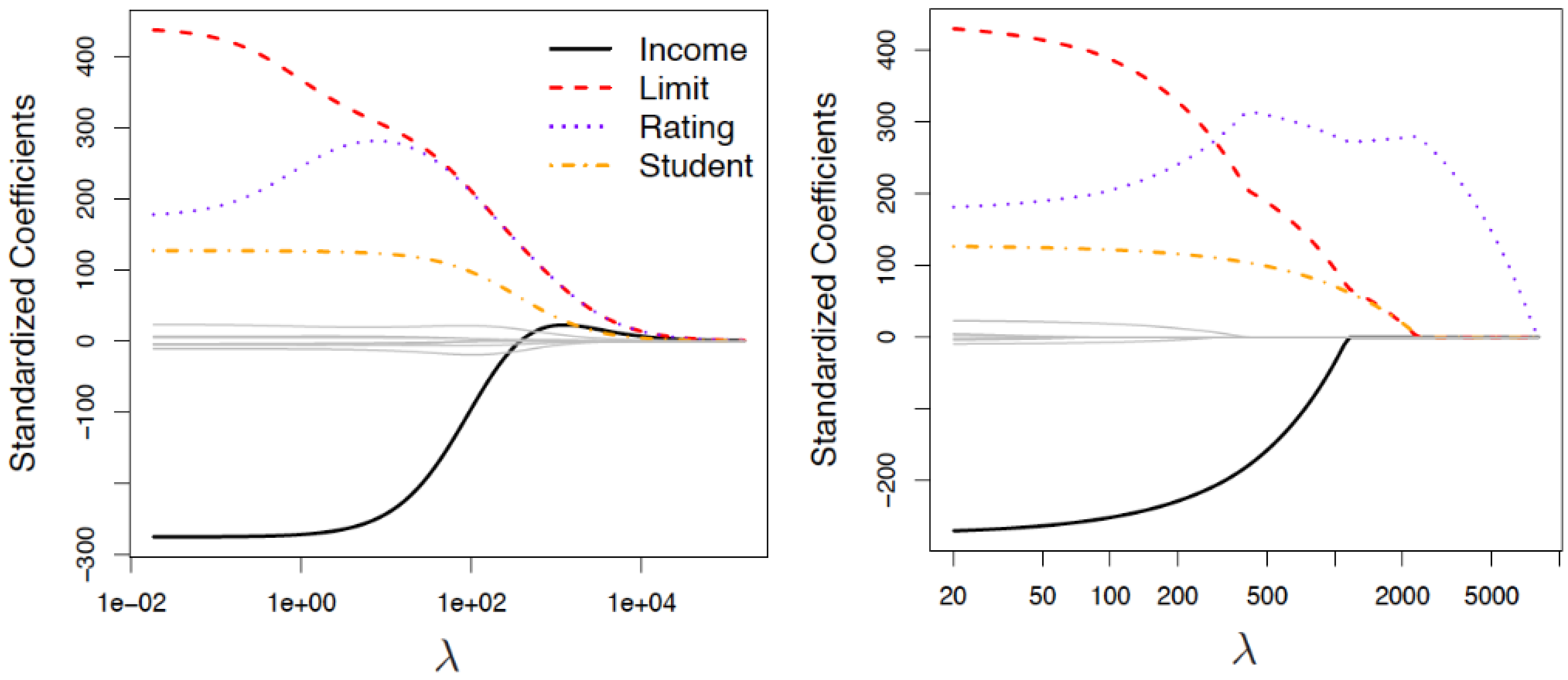
☺ **Can perform variable selection**

Example 5: Ridge vs. Lasso



lcp, age & gleason: the least important predictors → set to zero

Example 6: Ridge vs. Lasso



Constrained form of lasso & ridge

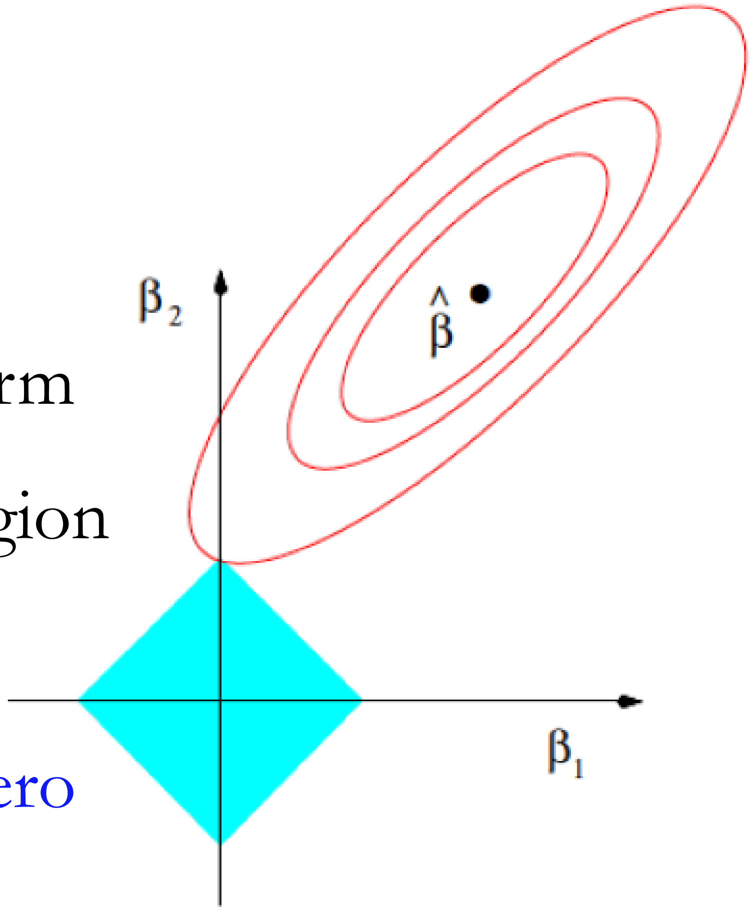
$$\hat{\beta}^{\text{ridge}} = \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \, \|y - X\beta\|_2^2 \quad \text{subject to } \|\beta\|_2^2 \leq t$$

$$\hat{\beta}^{\text{lasso}} = \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \, \|y - X\beta\|_2^2 \quad \text{subject to } \|\beta\|_1 \leq t$$

For any λ and corresponding solution in the penalized form, there is a value of t such that the above constrained form has this same solution. The imposed constraints constrict the coefficient vector to lie in some geometric shape centered around the origin

Type of shape (i.e., type of constraint) really matters!

Why lasso sets coefficients to zero?



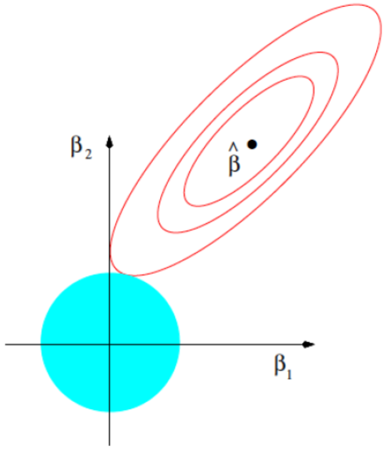
The elliptical contour plot represents sum of square error term

The diamond shape in the middle indicates the constraint region

Optimal point: intersection between ellipse & circle

- Corner of the diamond region, where the coefficient is zero

Instead with ridge:



Matlab code & examples

```
% Lasso regression

B = lasso(X,Y); % returns beta coefficients for a set of regularization parameters lambda
[B, I] = lasso(X,Y) % I contains information about the fitted models


% Fit a lasso model and let identify redundant coefficients
X = randn(100,5);                % 100 samples of 5 predictors
r = [0; 2; 0; -3; 0;];           % only two non-zero coefficients
Y = X*r + randn(100,1).*0.1;     % construct target using only two predictors
[B, I] = lasso(X,Y);             % fit lasso

% examining the 25th fitted model
B(:,25)         % beta coefficients
I.Lambda(25)    % lambda used
I.MSE(25)       % mean square error
```

Matlab code & examples

```
% Ridge regression

X = randn(100,5);                  % 100 samples of 5 predictors
r = [0; 2; 0; -3; 0;];             % only two non-zero coefficients
Y = X*r + randn(100,1).*0.1;       % construct target using only two predictors

model = fitrlinear(X,Y, ’Regularization’, ’ridge’, ‘Lambda’, 0.4));
predicted_Y = predict(model, X);    % predict Y, using the X data


err = mse(predicted_Y, Y);    % compute error

model.Beta     % fitted coefficients
```

3. Least Squares, Ridge Regression, and Overfitting

3.1 Goals

The goal of this exercise is to
- Implement and debug least-squares.
- Implement, debug and visualize basis function models.
- Understand overfitting.
- Implement Ridge regression.

3.2 Data and sample code

On the course website, you will find an archive `ex3code.zip`, which contains Matlab scripts and functions that you will need to finish this exercise. It also contains the dataset for this exercise. Download this file and extract it. Put it in the path of Matlab (if you don't know how to do this, refer to the Matlab guide from exercise session 1).

3.3 Least squares

Exercise 3.1 Implementing and debugging least squares.
- Implement the following function (in a new file `leastSquares.m`) which implements the solution of the normal equations as discussed in the class.

```
beta = leastSquares(y,tX)
```

  If you do not understand what `y` and `tX` are, refer to the previous exercise. Use the sample code shown in the lecture notes.
- To debug your code, you can use the output of the last exercise. Run gradient descent or grid search on the height-weight data from the last exercise, and make sure you get same value of $\boldsymbol{\beta}$ using both methods.
- Try various versions of least-square implementations given in the lecture notes. They must all give the same answer.

■

This is a useful method to debug your code, i.e. first implementing a simple method and then using it to check more complicated methods. If you have not finished exercise 2, please first finish implementing grid search method. If you are lagging behind, do not worry. You will get time later to catch up, but it is important that you finish previous exercises.

3.4 Least squares and basis function models

We will now implement and visualize a basis function model for the data `dataEx3.mat`.

As explained in the class, linear regression might not be suitable for nonlinear data. We will use polynomial basis functions to fit nonlinear data:

$$\phi_j(x) = x^j \tag{3.1}$$

Revise lecture notes. We will use different degree of polynomials, e.g. a two degree polynomial with x and x^2, a three degree polynomial with x,x^2 and x^3, etc. The higher degree polynomials are more expressive and can capture fine details in the data. Is that a good thing? Think about it.

To check the fit, we will use a measure called the Root-Mean-Square-Error (RMSE). It is related to MSE as follows:

$$\text{RMSE}(\boldsymbol{\beta}) = \sqrt{2 * \text{MSE}(\boldsymbol{\beta})} \tag{3.2}$$

MSE is difficult to interpret since it involves a square, therefore RMSE is a more interpretable measure. There are better measures like R^2 but you can learn about them from the book "Introduction to Statistical learning".

Let us now implement polynomial regressions and visualize their predictions.

Exercise 3.2 Implementing and visualizing polynomial regression.

- Run the script `visualize.m`. This script plots the data along with predictions using polynomial regression. In the provided script, the value of $\boldsymbol{\beta}$ is set to 0. Your goal is to find a good $\boldsymbol{\beta}$ using polynomial regression with degrees 1, 3, 7, and 12 respectively. You also need the function `computeCost.m` (for computation of RMSE, look inside the code). You wrote this function in the last exercise. You need to keep it in Matlab's path for your code to run (or copy the file over to this week's directory).
- Insert your function `leastSquares` in the script. You have to do this at two places.
- If the code runs successfully, you will see the data and the fit. You will clearly see why linear regression is not a good fit, while polynomial regression produces a better fit.
- Take a look at `myPoly.m` that we have provided with the code. What does it do? This code makes the $\boldsymbol{\Phi}$ matrix that we encountered in the lecture on Ridge Regression. Read the lecture notes and make sure you understand the function.
- If you look at the printed output of the script `visualize.m` (in Matlab's command window), you can see that RMSE decreases as we increase the degree of the polynomial. Does it mean that the fit gets better as we increase the degree? Which fit is the best in your view?

■

3.5 Evaluating model prediction performance

The answer to the last question should be clear if you followed the lecture. If not, discuss with others and clarify.

In practice, it matters that predictions are good for unseen examples, not only for training examples. To simulate the reality, we will now split our dataset into two parts: *training* and *testing*. We will fit the data using training data and compute RMSE on both test and training data.

Exercise 3.3 Train and test datasets.

- Run the script `trainTestSplit.m`. This script is supposed to show the train and test splits for various polynomial degrees. Again, the value of $\boldsymbol{\beta}$ is set to 0. You need to insert the function `leastSquares` in here.
- Insert `leastSquares.m`. If the code runs successfully, you will see RMSE

values printed for degrees 3, 7 and 12. For each degree, there are again three RMSE values which correspond to the following three splits of the data.
  - 90% training, 10% testing
  - 50% training, 50% testing
  - 10% training, 90% testing
- Look at the training and test RMSE for degree 3. Does this makes sense? Why? Discuss with others if you are unclear.
- Now look at RMSE for other two degrees. Do these make sense? Why? Discuss with others if you are unclear.
- Which split is better? Why? Refer to the lecture notes if unclear.
- To split the data, we use the function `split.m`. Look inside this function and understand how it works. Do you think that the order of samples is important when doing the split?
- The test RMSE for degree 12 is ridiculously high for the split 10%-90%. Why do you think this is the case? The answer lies in numerical inaccuracies. Make sure you understand this.
- **BONUS:** Imagine you have 5000 samples instead of 50. Which split might be better in that situation?

■

3.6 Ridge Regression

The previous exercise shows overfitting when using complex models. Let us now correct it using Ridge regression, as discussed in the class.

Exercise 3.4 Implementing and visualizing Ridge regression
- Write a function called `ridgeRegression.m`. The code should take the data as input, as well as the regularization parameter λ. Follow the equations derived in the lecture notes.

  `beta = ridgeRegression(y,tX,lambda)`
- You can debug your code by setting $\lambda = 0$. This should essentially give the same answer as least-squares code. You can also check that for large value of lambda, RMSE should be really bad.
- Choose a split of 50%-50% and plot train and test errors vs λ for polynomial degree 7. Follow the sample code given below. You should be able to reproduce the figure 3.1 shown below. Choose the value of λ using `logspace()`. Plot the error wrt λ using `semilogx()`

```
% given the split (yTr, XTr) and (yTe, XTe)
vals = logspace(-2,2,100)
for i = 1:length(vals)
    lambda = vals(i);
    % ridge regression
    [beta] = ridgeReg(yTr, XTr, lambda);
    % compute training error
    errTr(i) = computeCost(yTr, XTr, beta);
    % compute test error
    errTe(i) = computeCost(yTe, XTe, beta);
end
[errStar, lambdaStar] = min(errTe);
```

■

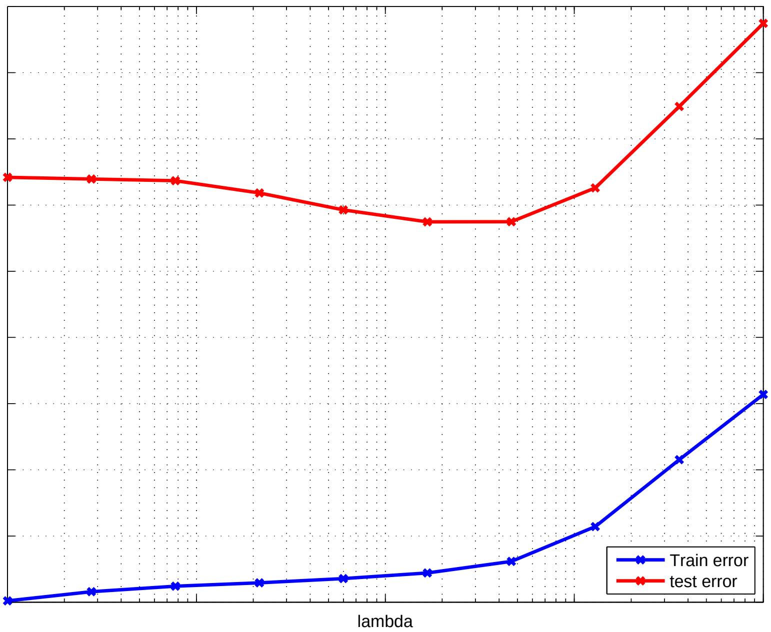


Figure 3.1: Effect of λ on training and test errors