Lecture 6: Linear Regression

Reading: Sections 3.2, 3.3

GU4241/GR5241 Statistical Machine Learning

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Multiple linear regression

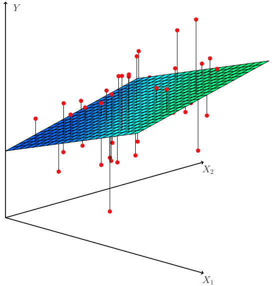

Figure 3.4

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$

$$\varepsilon \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

or, in matrix notation:

$$\mathbf{y} = \mathbf{X}\beta + \varepsilon,$$

where $\mathbf{y} = (y_1, \ldots, y_n)^T$, $\beta = (\beta_0, \ldots, \beta_p)^T$ and $\mathbf{X}$ is our usual data matrix with an extra column of ones on the left to account for the intercept.

The estimates $\hat{\beta}$

Our goal is to minimize the RSS (residual sum of squares, training error):

$$\begin{aligned}\text{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_{i,1} - \cdots - \beta_p x_{i,p})^2.\end{aligned}$$

This is minimized by the vector $\hat{\beta}$:

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.$$

This only exists when $\mathbf{X}^T\mathbf{X}$ is invertible. This requires $n \geq p$.

Multiple linear regression answers several questions

- Is at least one of the variables X_i useful for predicting the outcome Y?
- Which subset of the predictors is most important?
- How good is a linear model for these data?
- Given a set of predictor values, what is a likely value for Y, and how accurate is this prediction?

Testing whether a group of variables is important

- F-test:

  $$H_0 : \beta_{p-q+1} = \beta_{p-q+2} = \cdots = \beta_p = 0.$$

  RSS_0 is the residual sum of squares for the model in H_0.

  $$F = \frac{(\mathsf{RSS}_0 - \mathsf{RSS})/q}{\mathsf{RSS}/(n-p-1)}.$$

- Special case: $q = p$. Test whether any of the predictors are important.
- Special case: $q = 1$, exclude a single variable. Test whether this variable is important $\sim$ t-tests in R output. Must be careful with multiple testing.

Which subset of variables are important?

When choosing a subset of the predictors, we have 2^p choices. We cannot test every possible subset!

Instead we will use a **stepwise approach**:

1. Construct a sequence of p models with increasing number of variables.
2. Select the best model among them.

Three variants of stepwise selection

- **Forward selection:** Starting from a *null model*, include variables one at a time, minimizing the RSS at each step.
- **Backward selection:** Starting from the *full model*, eliminate variables one at a time, choosing the one with the largest t-test p-value at each step.
- **Mixed selection:** Starting from a *null model*, include variables one at a time, minimizing the RSS at each step. If the p-value for some variable goes beyond a threshold, eliminate that variable.

Which subset of variables are important?

The output of a stepwise selection method is a range of models:

- $\{\}$
- $\{\texttt{tv}\}$
- $\{\texttt{tv}, \texttt{newspaper}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}, \texttt{facebook}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}, \texttt{facebook}, \texttt{twitter}\}$

6 choices are better than $2^6 = 64$. We use different *tuning methods* to decide which model to use; e.g. cross-validation, AIC, BIC.

Which subset of variables are important?

When choosing a subset of the predictors, we have 2^p choices.

- **Forward selection:** Starting from a *null model*, include variables one at a time, minimizing the RSS at each step.
- **Backward selection:** Starting from the *full model*, eliminate variables one at a time, choosing the one with the largest p-value at each step.
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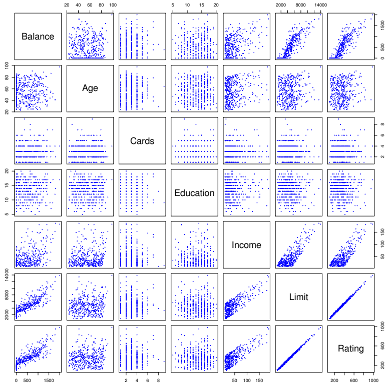
Dealing with categorical or qualitative predictors

Example: Credit dataset



In addition, there are 4 qualitative variables:

- `gender`: male, female.
- `student`: student or not.
- `status`: married, single, divorced.
- `ethnicity`: African American, Asian, Caucasian.

Dealing with categorical or qualitative predictors

For each qualitative predictor, e.g. `ethnicity`:

- Choose a baseline category, e.g. African American
- For every other category, define a new predictor:
  - X_{Asian} is 1 if the person is Asian and 0 otherwise.
  - $X_{\text{Caucasian}}$ is 1 if the person is Caucasian and 0 otherwise.

The model will be:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_7 X_7 + \beta_{\text{Asian}} X_{\text{Asian}} + \beta_{\text{Caucasian}} X_{\text{Caucasian}} + \varepsilon.$$

β_{Asian} is the relative effect on `balance` for being Asian compared to the baseline category.

Dealing with categorical or qualitative predictors

- The model fit and predictions are independent of the choice of the baseline category.
- However, hypothesis tests derived from these variables are affected by the choice.
  - **Solution:** To check whether `ethnicity` is important, use an F-test for the hypothesis $\beta_{\text{Asian}} = \beta_{\text{Caucasian}} = 0$. This does not depend on the coding.
- Other ways to encode qualitative predictors produce the same fit $\hat{f}$, but the coefficients have different interpretations.

How good are the predictions?

The function `predict` in R output predictions from a linear model; eg. $x_0 = (5, 10, 15)$:

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
       interval="confidence")
    fit   lwr   upr
1 29.80 29.01 30.60
2 25.05 24.47 25.63
3 20.30 19.73 20.87
```

"Confidence intervals" reflect the uncertainty on $\hat{\beta}$; ie. confidence interval for $\hat{f}(x_0)$.

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
       interval="prediction")
    fit    lwr   upr
1 29.80 17.566 42.04
2 25.05 12.828 37.28
3 20.30  8.078 32.53
```

"Prediction intervals" reflect uncertainty on $\hat{\beta}$ and the irreducible error ε as well; i.e. confidence interval for y_0.

Recap

So far, we have:

- Defined Multiple Linear Regression
- Discussed how to test the importance of variables.
- Described one approach to choose a subset of variables.
- Explained how to code qualitative variables.
- Now, how do we evaluate model fit? Is the linear model any good? What can go wrong?

How good is the fit?

To assess the fit, we focus on the residuals.

- $R^2 = \text{Corr}^2(Y, \hat{Y})$, always increases as we add more variables.
- The residual standard error (RSE) does not always improve with more predictors:

$$\text{RSE} = \sqrt{\frac{1}{n-p-1}\text{RSS}}.$$

- **Visualizing the residuals** can reveal phenomena that are not accounted for by the model.

Potential issues in linear regression

1. Interactions between predictors
2. Non-linear relationships
3. Correlation of error terms
4. Non-constant variance of error (heteroskedasticity).
5. Outliers
6. High leverage points
7. Colinearity

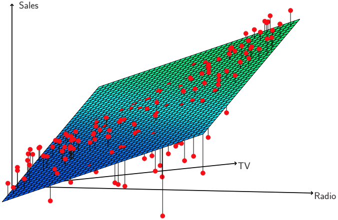
Interactions between predictors

Linear regression has an *additive* assumption:

$$\texttt{sales} = \beta_0 + \beta_1 \times \texttt{tv} + \beta_2 \times \texttt{radio} + \varepsilon$$

i.e. An increase of $100 dollars in TV ads causes a fixed increase in sales, regardless of how much you spend on radio ads.

If we visualize the residuals, it is clear that this is false:



Interactions between predictors

One way to deal with this is to include multiplicative variables in the model:

$$\texttt{sales} = \beta_0 + \beta_1 \times \texttt{tv} + \beta_2 \times \texttt{radio} + \beta_3 \times (\texttt{tv} \cdot \texttt{radio}) + \varepsilon$$

The **interaction variable** is high when both `tv` and `radio` are high.

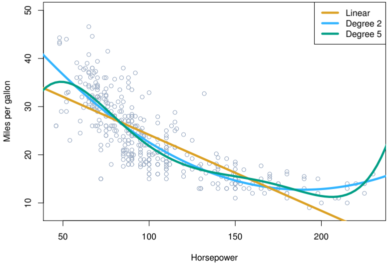
Interactions between predictors

R makes it easy to include interaction variables in the model:

```
> lm.fit=lm(Sales~.+Income:Advertising+Price:Age,data=Carseats)
> summary(lm.fit)

Call:
lm(formula = Sales ~ . + Income:Advertising + Price:Age, data =
     Carseats)

Residuals:
   Min      1Q  Median      3Q     Max
-2.921  -0.750   0.018   0.675   3.341

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)         6.575565   1.008747    6.52  2.2e-10 ***
CompPrice           0.092937   0.004118   22.57  < 2e-16 ***
Income              0.010894   0.002604    4.18  3.6e-05 ***
Advertising         0.070246   0.022609    3.11  0.00203 **
Population          0.000159   0.000368    0.43  0.66533
Price              -0.100806   0.007440  -13.55  < 2e-16 ***
ShelveLocGood       4.848676   0.152838   31.72  < 2e-16 ***
ShelveLocMedium     1.953262   0.125768   15.53  < 2e-16 ***
Age                -0.057947   0.015951   -3.63  0.00032 ***
Education          -0.020852   0.019613   -1.06  0.28836
UrbanYes            0.140160   0.112402    1.25  0.21317
USYes              -0.157557   0.148923   -1.06  0.29073
Income:Advertising  0.000751   0.000278    2.70  0.00729 **
Price:Age           0.000107   0.000133    0.80  0.42381
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Non-linearities

Example: Auto dataset.



A scatterplot between a predictor and the response may reveal a non-linear relationship.

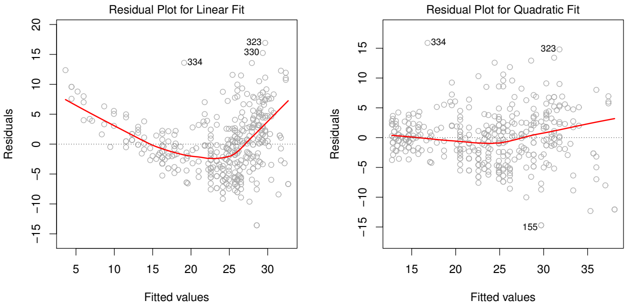
Solution: include polynomial terms in the model.

$$\begin{aligned}
\texttt{MPG} = \beta_0 + \beta_1 \times \texttt{horsepower} + \varepsilon \\
+ \beta_2 \times \texttt{horsepower}^2 + \varepsilon \\
+ \beta_3 \times \texttt{horsepower}^3 + \varepsilon \\
+ \ldots + \varepsilon
\end{aligned}$$

Non-linearities

In 2 or 3 dimensions, this is easy to visualize. What do we do when we have too many predictors?

Plot the residuals against the *response* and look for a pattern:



Correlation of error terms

We assumed that the errors for each sample are independent:

$$y_i = f(x_i) + \varepsilon_i \quad ; \quad \varepsilon_i \sim \mathcal{N}(0, \sigma) \text{ i.i.d.}$$

What if this breaks down?

The main effect is that this invalidates any assertions about Standard Errors, confidence intervals, and hypothesis tests:

Example: Suppose that by accident, we double the data (we use each sample twice). Then, the standard errors would be artificially smaller by a factor of $\sqrt{2}$.

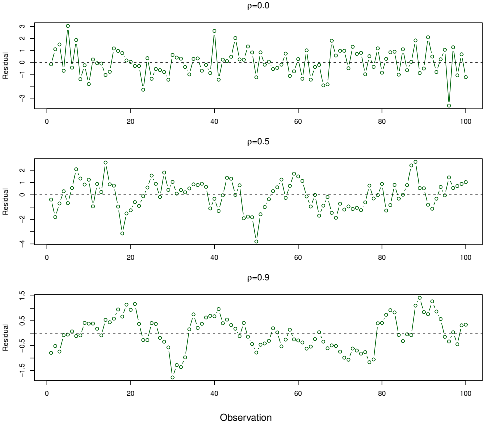
Correlation of error terms

When could this happen in real life:

- **Time series:** Each sample corresponds to a different point in time. The errors for samples that are close in time are correlated.
- **Spatial data:** Each sample corresponds to a different location in space.
- Study on predicting height from weight at birth. Suppose some of the subjects in the study are in the same family, their shared environment could make them deviate from $f(x)$ in similar ways.

Correlation of error terms

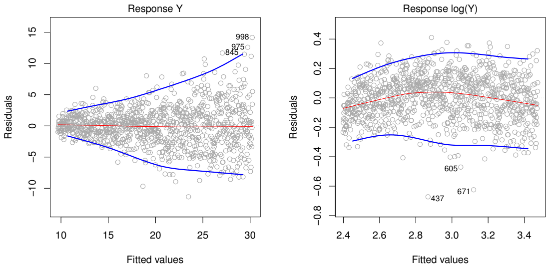
Simulations of time series with increasing correlations between ε_i.



Non-constant variance of error (heteroskedasticity)

The variance of the error depends on the input.

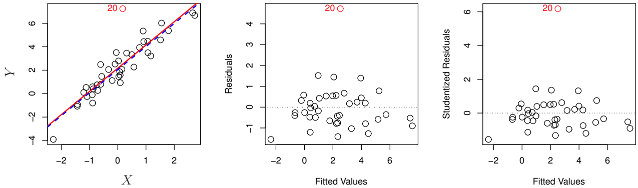
To diagnose this, we can plot residuals vs. fitted values:



Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.

Outliers

Outliers are points with very high errors.



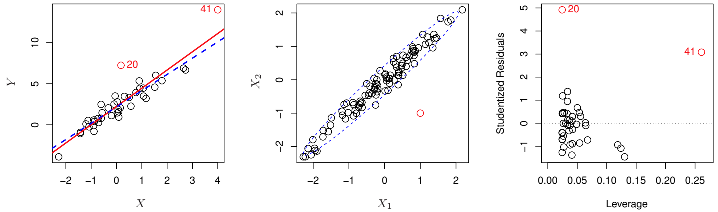
While they may not affect the fit, they might affect our assessment of model quality.

Possible solutions:

- If we believe an outlier is due to an error in data collection, we can remove it.
- An outlier might be evidence of a missing predictor, or the need to specify a more complex model.

High leverage points

Some samples with extreme inputs have an outsized effect on $\hat{\beta}$.



This can be measured with the **leverage statistic** or **self influence**:

$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = (\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)_{i,i} \in [1/n, 1].$$

High leverage points

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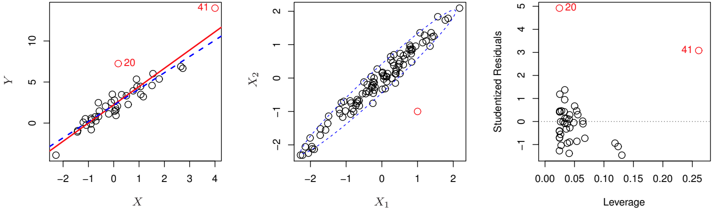

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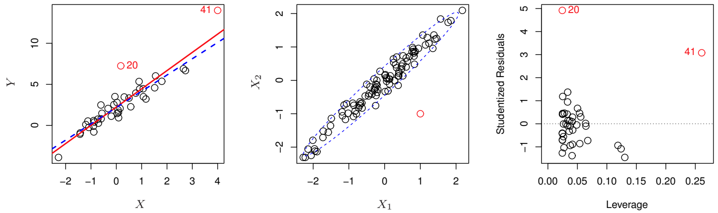
$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = (\underbrace{\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T}_{\text{Hat matrix}})_{i,i} \in [1/n, 1].$$

Studentized residuals

- The residual $\hat{\epsilon}_i = y_i - \hat{y}_i$ is an estimate for the noise ϵ_i.
- The standard error of $\hat{\epsilon}_i$ is $\sigma\sqrt{1 - h_{ii}}$.
- A **studentized residual** is $\hat{\epsilon}_i$ divided by its standard error.
- It follows a Student-t distribution with $n - p - 2$ degrees of freedom.

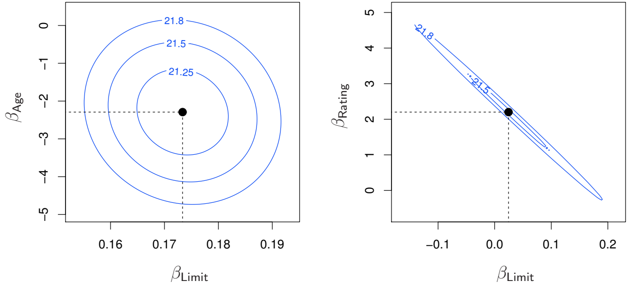


Collinearity

Problem: The coefficients become *unidentifiable*. Consider the extreme case of using two identical predictors `limit`:

$$\begin{aligned}\texttt{balance} &= \beta_0 + \beta_1 \times \texttt{limit} + \beta_2 \times \texttt{limit} \\ &= \beta_0 + (\beta_1 + 100) \times \texttt{limit} + (\beta_2 - 100) \times \texttt{limit}\end{aligned}$$

The fit $(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)$ is just as good as $(\hat{\beta}_0, \hat{\beta}_1 + 100, \hat{\beta}_2 - 100)$.



Collinearity

If 2 variables are collinear, we can easily diagnose this using their correlation.

A group of q variables is **multilinear** if these variables "contain less information" than q independent variables. Pairwise correlations may not reveal multilinear variables.

The Variance Inflation Factor (VIF) measures how *necessary* a variable is, or how predictable it is given the other variables:

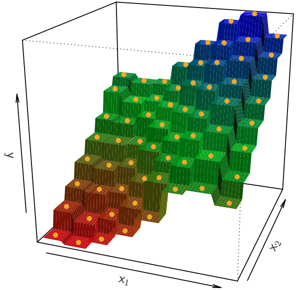
$$VIF(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}},$$

where $R^2_{X_j|X_{-j}}$ is the R^2 statistic for Multiple Linear regression of the predictor X_j onto the remaining predictors.

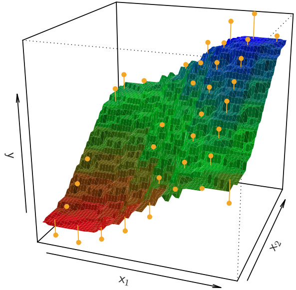
Comparing Linear Regression to K-nearest neighbors

Linear regression: prototypical parametric method.
KNN regression: prototypical nonparametric method.

$$\hat{f}(x) = \frac{1}{K} \sum_{i \in N_K(x)} y_i$$



$K = 1$



$K = 9$

Comparing Linear Regression to K-nearest neighbors

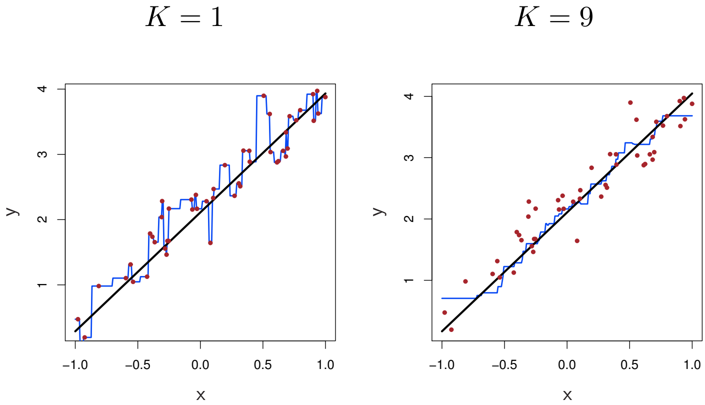
Linear regression: prototypical parametric method.

KNN regression: prototypical nonparametric method.

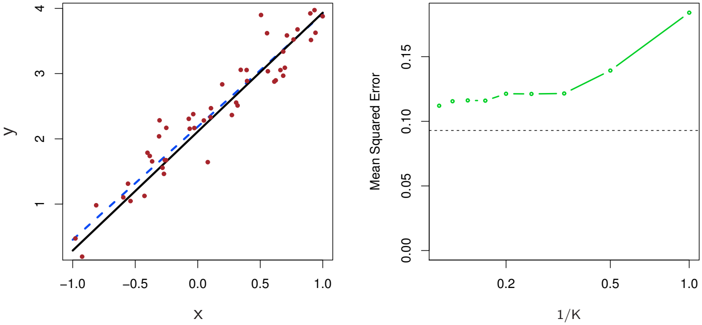
Long story short:

- KNN is only better when the function f is not linear.
- When n is not much larger than p, even if f is nonlinear, Linear Regression can outperform KNN. KNN has smaller bias, but this comes at a price of higher variance.

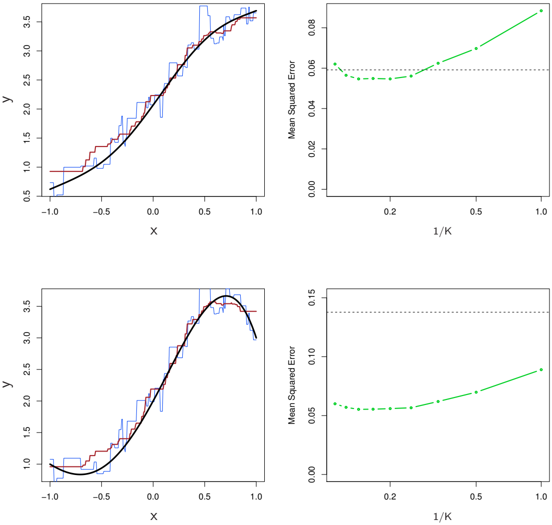
KNN estimates for a simulation from a linear model



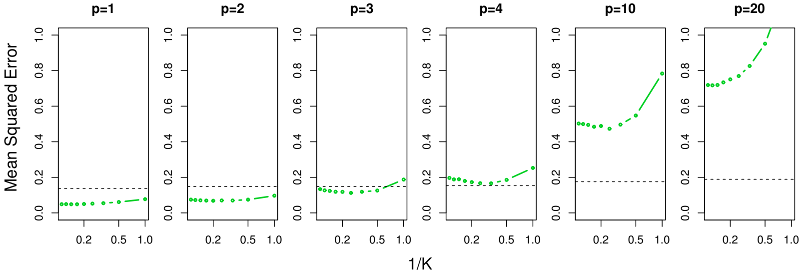
Linear models dominate KNN



Increasing deviations from linearity



When there are more predictors than observations, Linear Regression dominates



When $p \gg n$, each sample has no nearest neighbors, this is known as the *curse of dimensionality*. The variance of KNN regression is very large.

Next time: Classification

Supervised learning with a **qualitative or categorical** response.

Just as common, if not more common than regression:

- *Medical diagnosis:* Given the symptoms a patient shows, predict which of 3 conditions they are attributed to.
- *Online banking:* Determine whether a transaction is fraudulent or not, on the basis of the IP address, client's history, etc.
- *Web searching:* Based on a user's history, location, and the string of a web search, predict which link a person is likely to click.
- *Online advertising:* Predict whether a user will click on an ad or not.