Scientific Computing for Biologists

Linear Algebra Review II & Regression

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Overview of Lecture

- More Linear Algebra
  - Linear combinations and Spanning Spaces
  - Subspaces
  - Basis vectors
  - Dimension
  - Rank
- More on Regression
  - Multiple regression
  - Curvilinear regression
  - Logistic regression
  - Major axis regression

Hands-on Session

- Regression in R
- Multiple regression
- Logistic regression
- Locally weighted regression (LOESS or LOWESS)

Space Spanned by a List of Vectors

Definition

Let X be a finite list of n-vectors. The **space spanned** by X is the set of all vectors that can be written as linear combinations of the vectors in X.

A space spanned includes the zero vector and is closed under addition and multiplication by a scalar.

Remember that a *linear combination* of vectors is an equation of the form $z = b_1x_1 + b_2x_2 + \cdots + b_px_p$

Subspaces

$\mathbb{R}^n$ denotes the seat of real n-vectors - the set of all $n \times 1$ matrices with entries from the set $\mathbb{R}$ of real numbers.

Definition

A **subspace** of $\mathbb{R}^n$ is a subset S of $\mathbb{R}^n$ with the following properties:

1. $0 \in S$
2. If $u \in S$ then $ku \in S$ for all real numbers k
3. If $u \in S$ and $v \in S$ then $u + v \in S$

Examples of subspaces of $\mathbb{R}^n$:

- any space spanned by a list of vectors in $\mathbb{R}^n$
- the set of all solution to an equation $Ax = 0$ where A is a $p \times n$ matrix, for any number p.

Basis

Let S be a subspace of $\mathbb{R}^n$. Then there is a finite list, X of vectors from S such that S is the space spanned by X.

Let S be a subspace of $\mathbb{R}^n$ spanned by the list $(u_1, u_2, \ldots, u_n)$. Then there is a linearly independent sublist of $(u_1, u_2, \ldots, u_n)$ that also spans S.

Definition

A list X is a **basis** for S if:

- X is linearly independent
- S is the subspace spanned by X

Dimension

Let S be a subspace of $\mathbb{R}^n$.

Definition

The **dimension** of S is the number of elements in a basis for S.

Rank of a Matrix

Let A by an $n \times p$ matrix.

Definition

The **rank** of A is equal to the dimension of the row space of A which is equal to the dimension of the column space of A.

Where the row space of A is the space spanned by the list of rows of A and the column space of A is defined similarly.

Equivalence Theorem

Let A by an $p \times p$ matrix. The following are equivalent

- A is singular
- the rank of A is less than p
- the columns of A form a LD list in $\mathbb{R}^n$.
- the rows of A form a LD list in $\mathbb{R}^n$
- the equation $Ax = 0$ has non-trivial solutions
- the determinant of A is zero

Regression Models

Variable space view of multiple regression

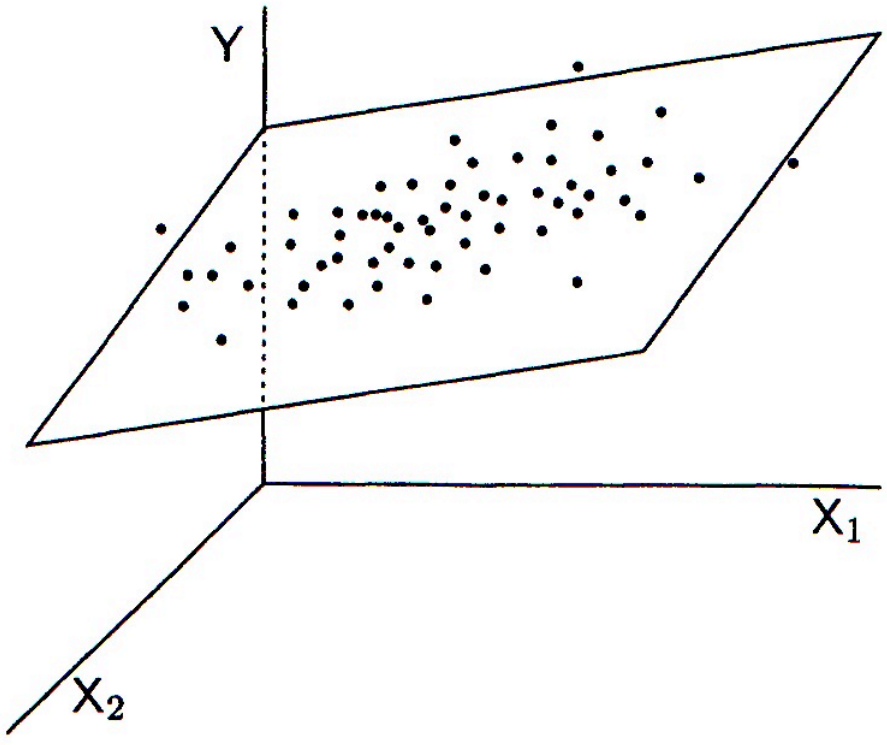
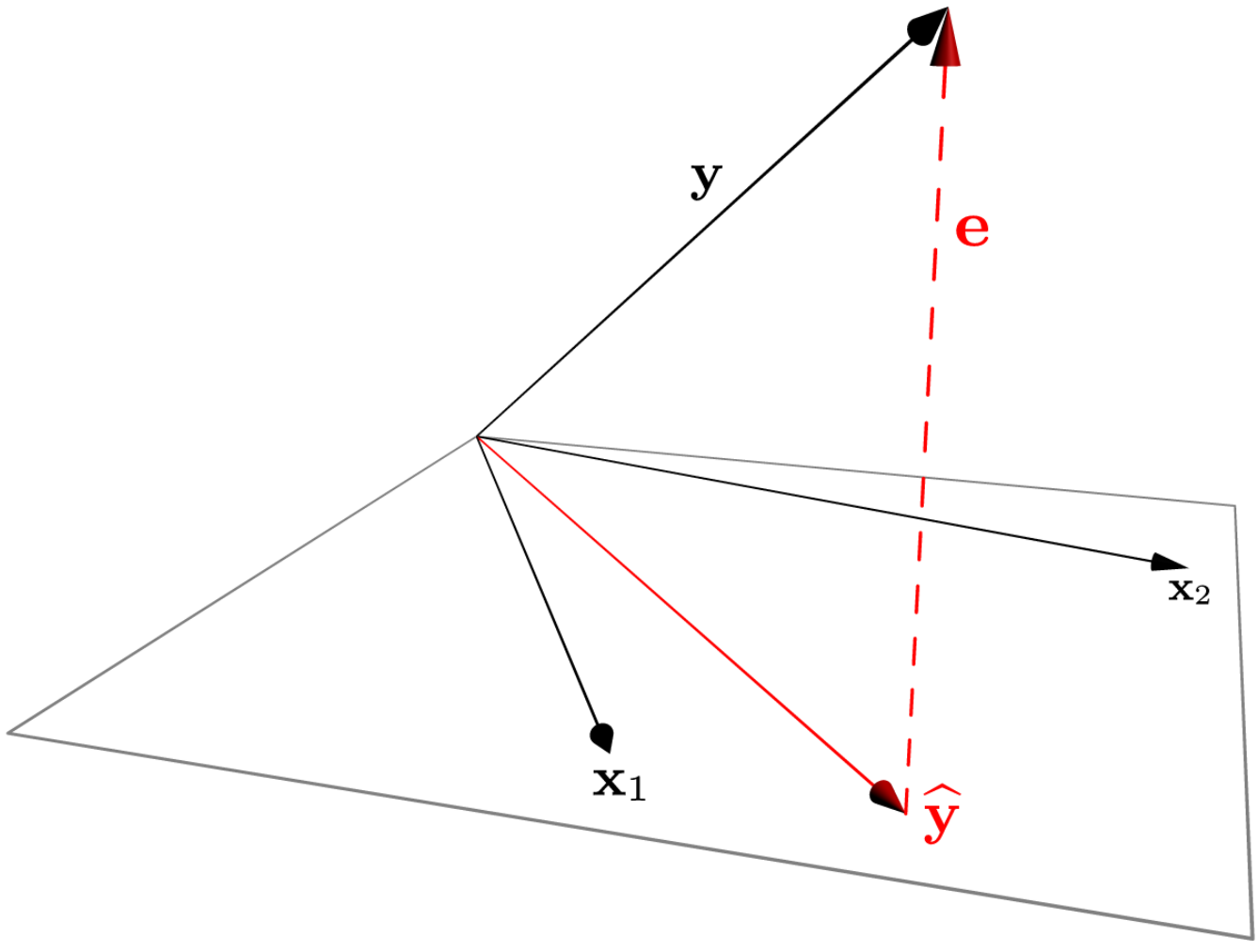


Figure 4.1: *The regression of* Y *onto* X_1 *and* X_2 *as a scatterplot in variable space.*

Subject Space Geometry of Multiple Regression



Multiple Regression

Let Y be a vector of values for the outcome variable. Let X_i be explanatory variables and let x_i be the mean-centered explanatory variables.

$$Y = \hat{Y} + e$$

where –

Uncentered version:

$$\hat{Y} = a1 + b_1X_1 + b_2X_2 + \cdots + b_pX_p$$

Centered version:

$$\hat{y} = b_1x_1 + b_2x_2 + \cdots + b_px_p$$

Statistical Model for Multiple Regression

In matrix form:

$$y = Xb + e$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix};$$

$$b = \begin{bmatrix} a \\ b_1 \\ b_2 \\ \vdots \\ b_p \end{bmatrix}; e = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

Estimating the Coefficients for Multiple Regression

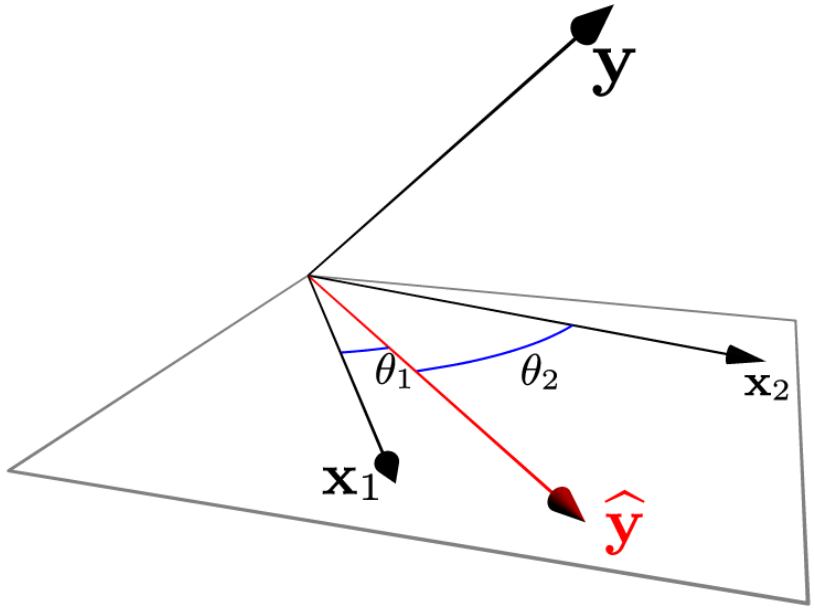
$$y = Xb + e$$

Estimate b as:

$$b = (X^T X)^{-1} X^T y$$

Multiple Regression Loadings

The regression **loadings** should be examined as well as the regression coefficients.



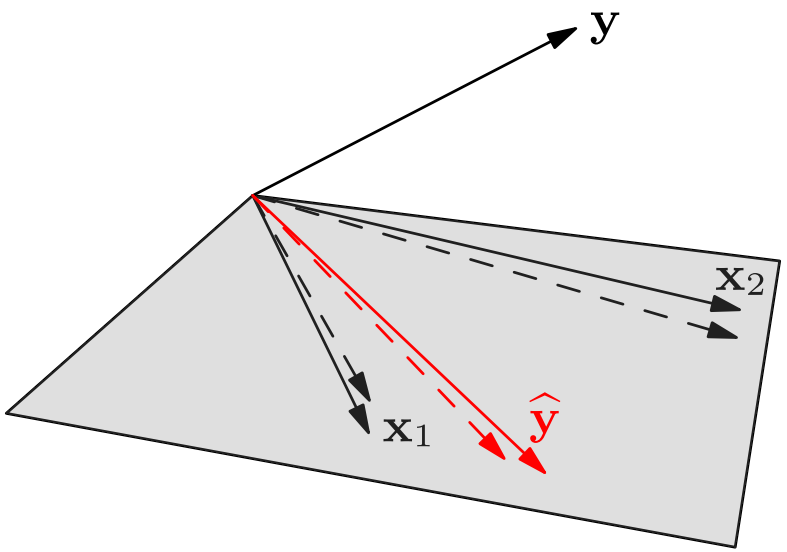
Loadings are given by:

$$\cos\theta_{\vec{x_j},\vec{\hat{y}}} = \frac{\vec{x_j}\cdot\vec{\hat{y}}}{|\vec{x_j}||\vec{\hat{y}}|}$$

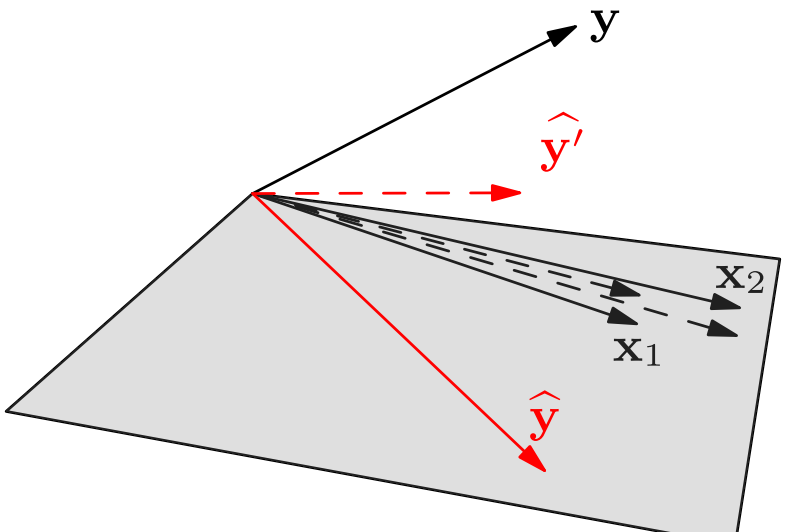
Multiple regression: Cautions and Tips

- Comparing the size of regression coefficients only makes sense if all the predictor variables have the same scale
- The predictor variables (columns of X) must be linearly independent; when they're not the variables are **multicollinear**
- Predictor variables that are **nearly multicollinear** are, perhaps, even more difficult to deal with

Why is near multicollinearity of the predictors a problem?



(a) Non-collinear predictors



What can I do if my predictors are (nearly) collinear?

- Drop some of the linearly dependent sets of predictors.
- Replace the linearly dependent predictors with a combined variable.
- Define orthogonal predictors, via linear combinations of the original variables (PC regression approach)
- 'Tweak' the predictor variables so that they're no longer multicollinear (Ridge regression).

Curvilinear Regression

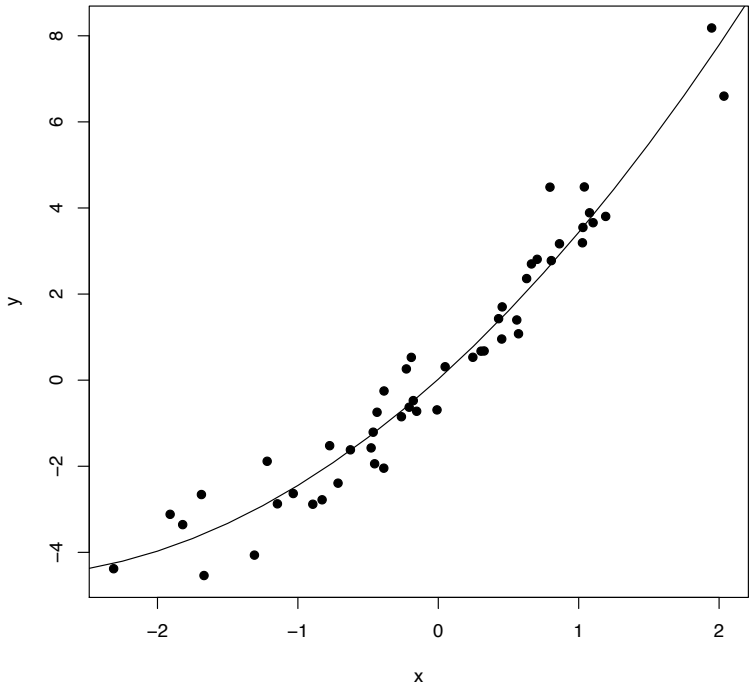
Curvilinear regression using **polynomial models** is simply multiple regression with the x_i replace by powers of x.

$$\hat{y} = b_1 x + b_2 x^2 + \cdots + b_p x^n$$

Note:

- this is still a *linear* regression (linear in the coefficients)
- best applied when a specific hypothesis justifies there use
- generally not higher than quadratic or cubic

Example of Curvilinear Regression

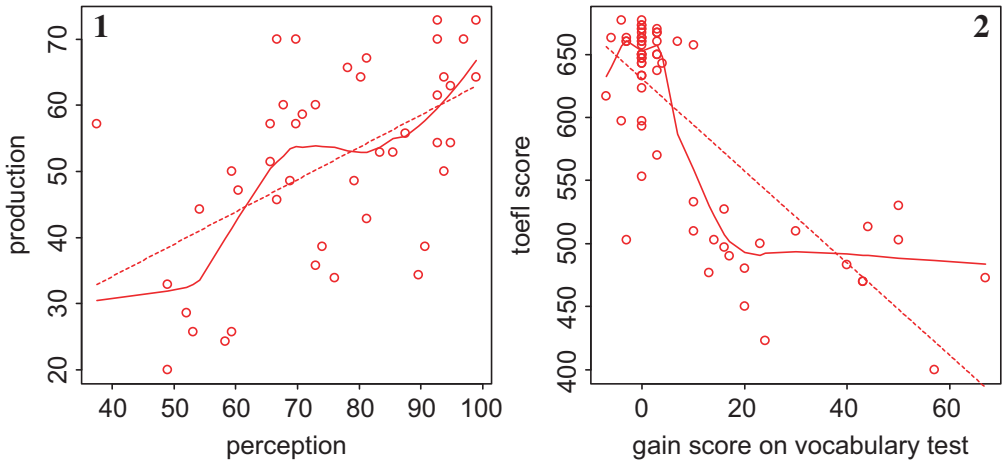


$$y = 3x + 0.5x^2 + e$$

```
lm(formula = y ~ x + I(x^2))
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.02229    0.11651   0.191    0.849
x            2.94001    0.09693  30.331  < 2e-16 ***
I(x^2)       0.47146    0.07685   6.135 1.68e-07 ***
```

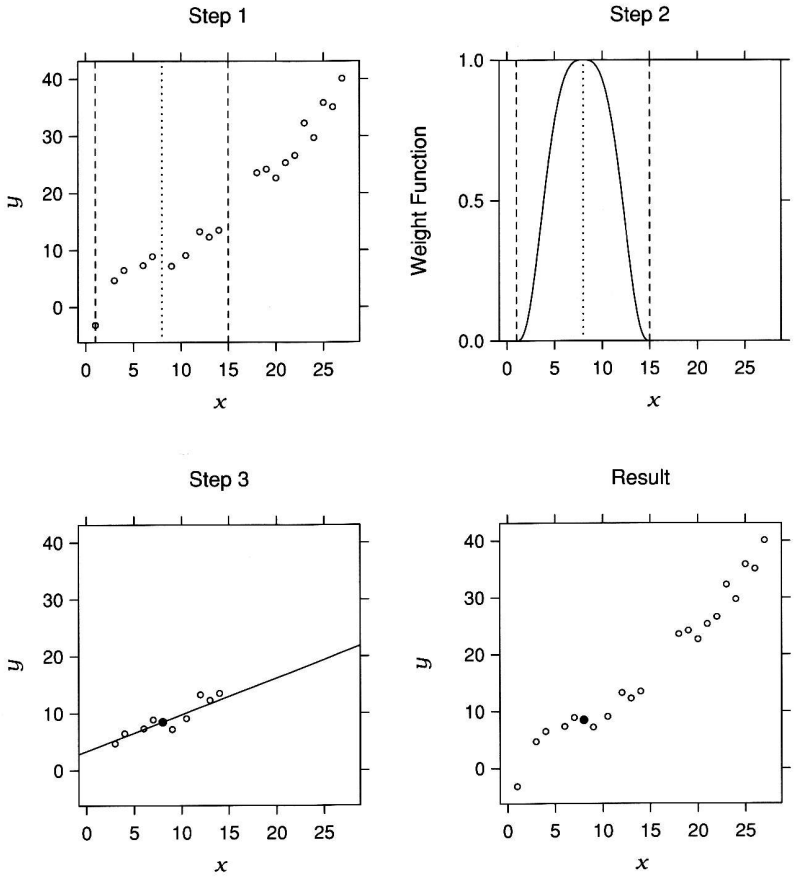
Loess Regression

- A type of non-parametric regression
- Basic idea – fit a curve (or surface) to a set of data by fitting a large number of *local regressions*.
- Cleveland, W.S. (1979). “Robust Locally Weighted Regression and Smoothing Scatterplots". Journal of the American Statistical Association 74 (368): 829-836. doi:10.2307/2286407.



Graphical overview of Loess fitting, I

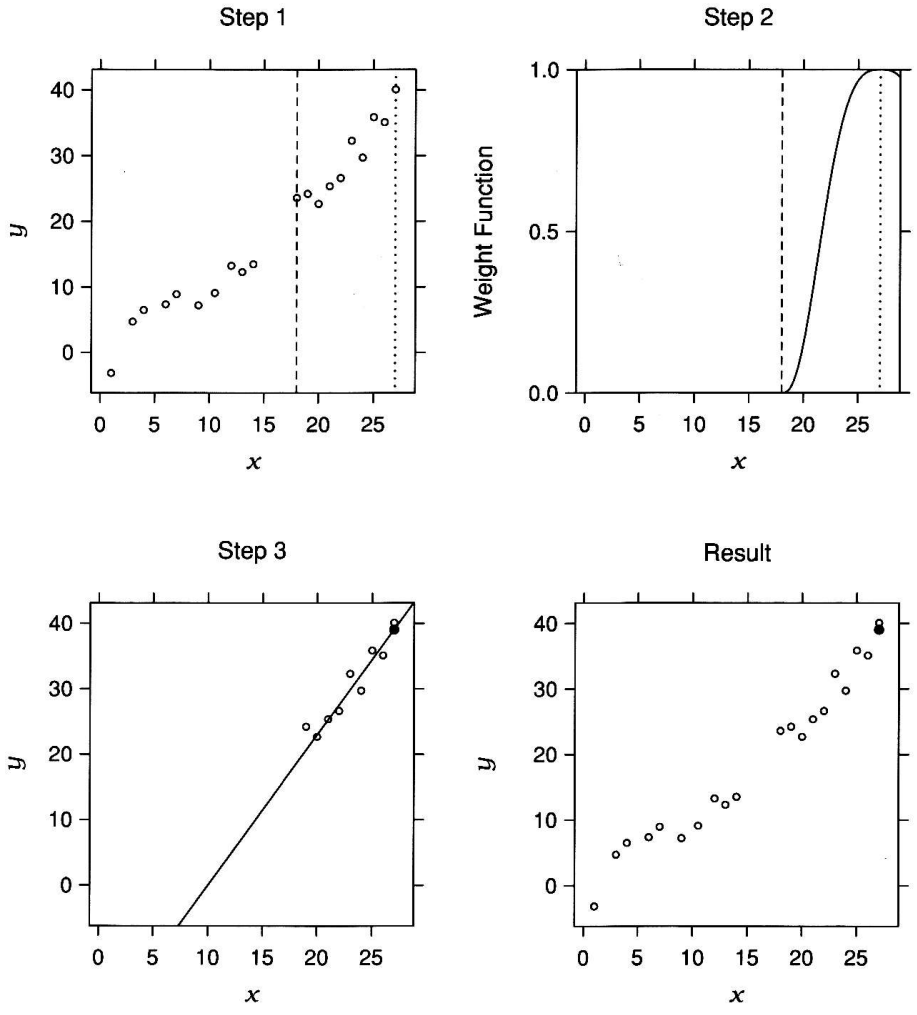
from Cleveland (1993)



3.49 HOW LOESS WORKS. The graphs show how the initial fit at $x = 8$ is computed. (Top left) α, which is 0.5, is multiplied by 20, the number of points, which gives 10. A vertical strip is defined around $x = 8$ so that one boundary is at the 10th nearest neighbor. (Top right) Weights are defined for the points using the weight function. (Bottom left) A line is fitted using weighted least-squares. The value of the line at $x = 8$ is the initial loess fit at $x = 8$. (Bottom right) The result is one point of the initial loess curve, shown by the filled circle.

Graphical overview of Loess fitting, II

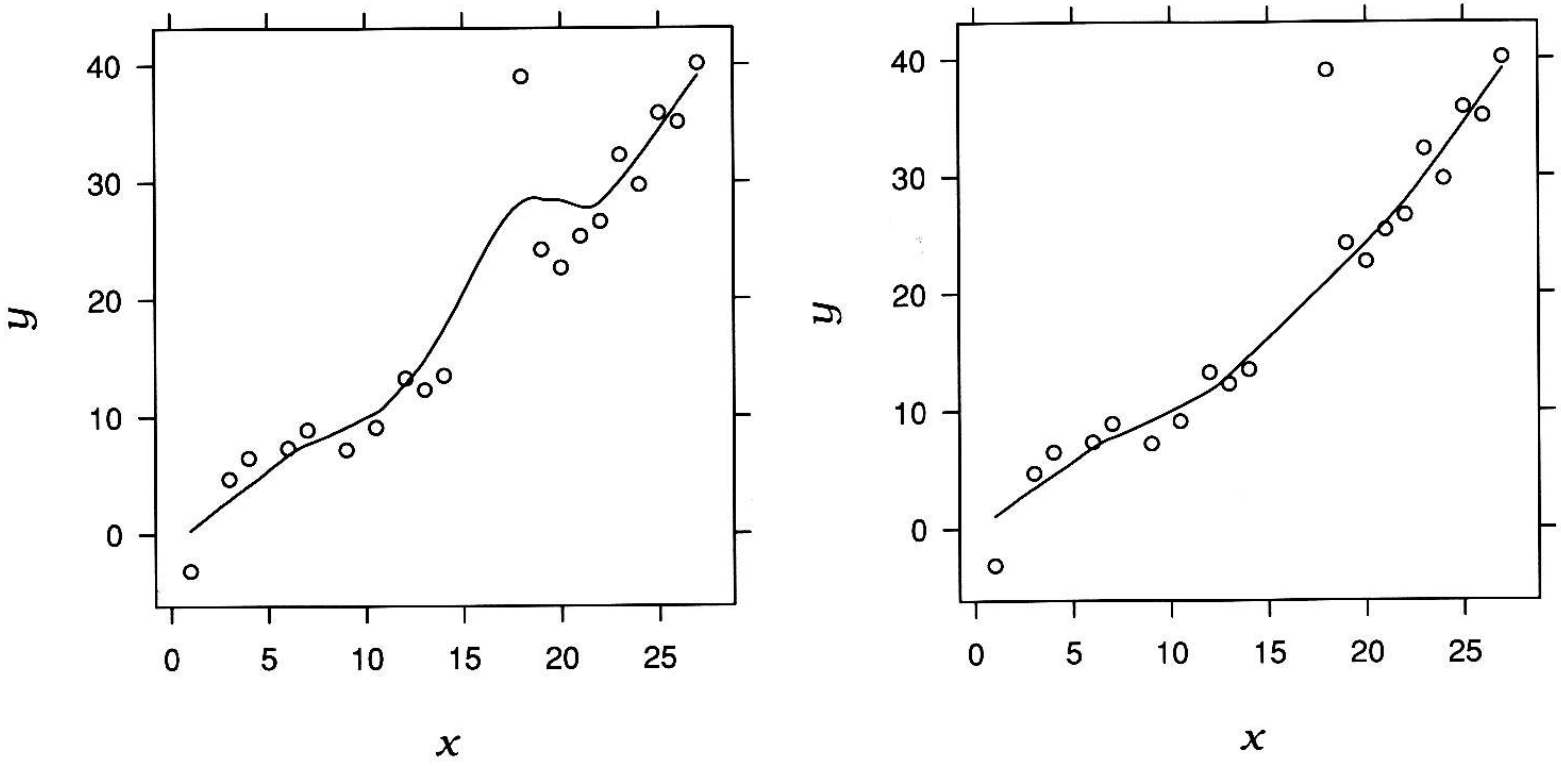
from Cleveland (1993)



3.50 HOW LOESS WORKS. The computation of the initial loess fit value at $x = 27$ is illustrated.

Graphical overview of Loess fitting, III

from Cleveland (1993)



3.51 HOW LOESS WORKS. Loess employs robustness iterations that prevent outliers from distorting the fit. (Left panel) The open circles are the points of the graph; there is one outlier between $x = 15$ and $x = 20$. The initial loess curve has been distorted in the neighborhood of the outlier. (Right panel) The graphed curve is the fit after four robustness iterations. Now the fit follows the general pattern of the data.

Logistic Regression

Logistic regression is used when the dependent variable is discrete (often binary). The explanatory variables may be either continuous or discrete.

Examples:

- whether a gene is turned off (=0) or on (=1) as a function of levels of various proteins
- whether an individual is healthy (=0) or diseased (=1) as a function of various risk factors.

Model the binary responses as:

$$P(Y = 1|X_1, \ldots, X_p) = g^{-1}(\beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)$$

So we're modeling the probability of the states as a function of a linear combination of the predictor variables.

Logistic Regression, Logit Transform

Most common choice for g is the 'logit link' function:

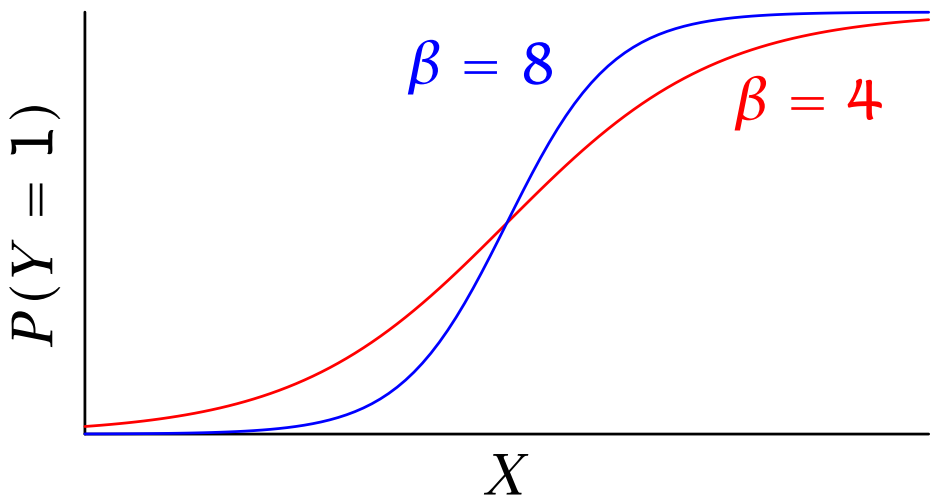
$$g(\pi) = log\left(\frac{\pi}{1-\pi}\right)$$

and g^{-1} is thus the logistic function:

$$g^{-1}(z) = \frac{e^z}{1+e^z}$$

Logistic Regression

$$P(Y = 1|X) = \frac{e^{X\beta}}{1 + e^{X\beta}}$$



Notes on Logistic Regression

- The regression is no longer linear
- Estimating the β in logistic regression is done via maximum likelihood estimation (MLE)
- Information-theoretic metrics of model fit rather than F-statistics

Logistic Regression Example

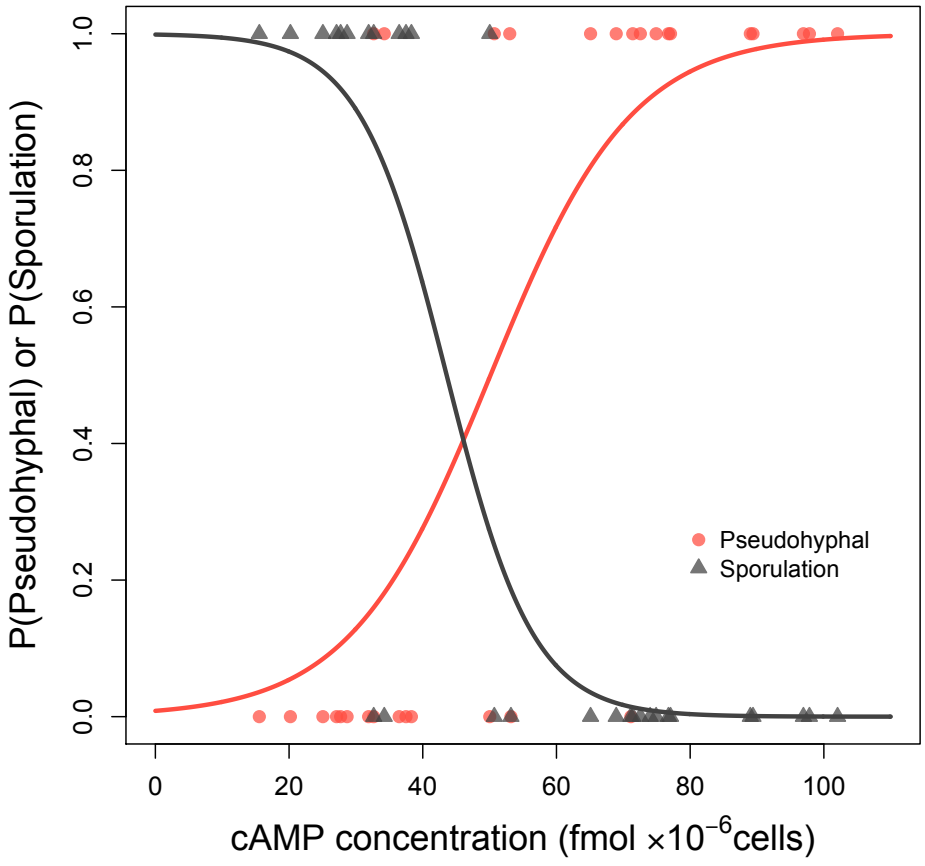
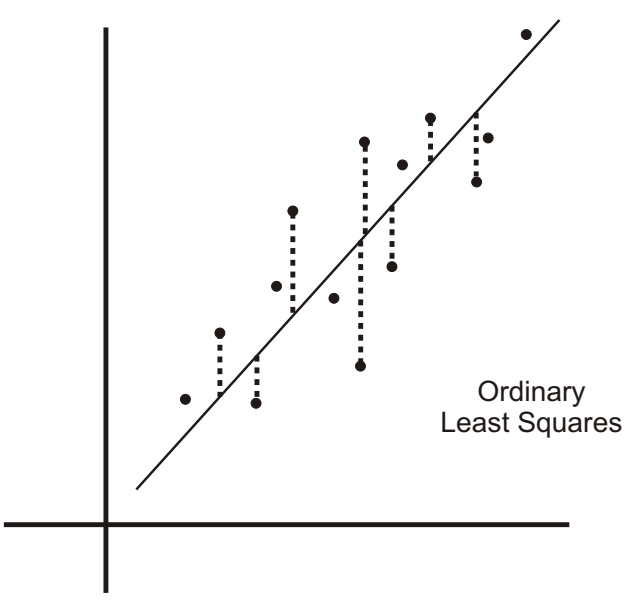
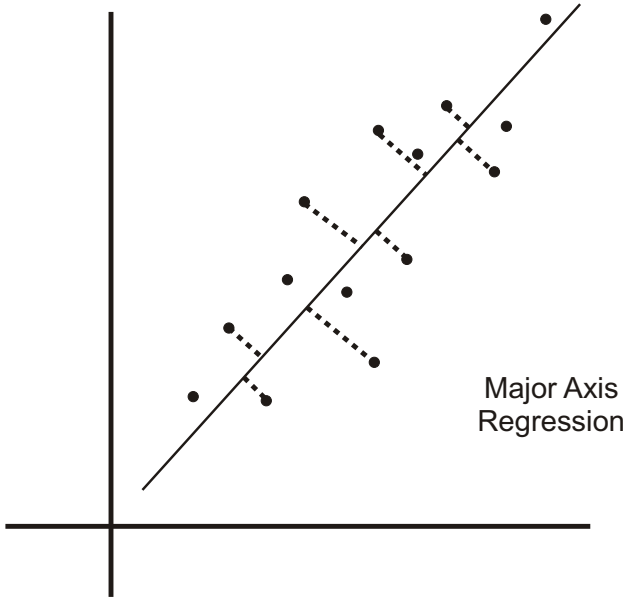


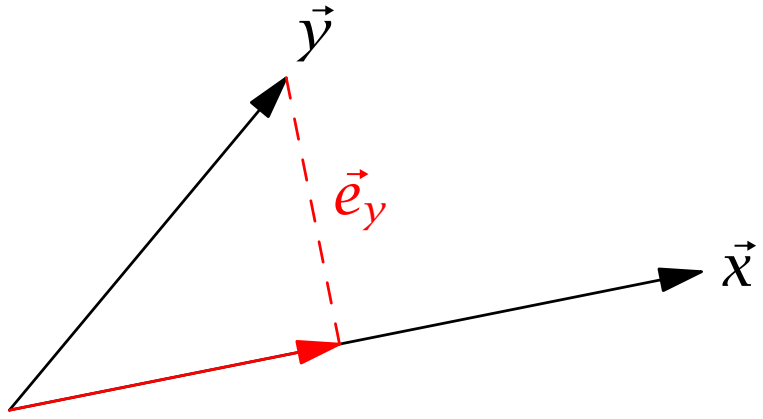
Figure: Logistic regression for yeast developmental phenotypes as a function of cAMP concentration.

OLS vs. Major Axis Regression

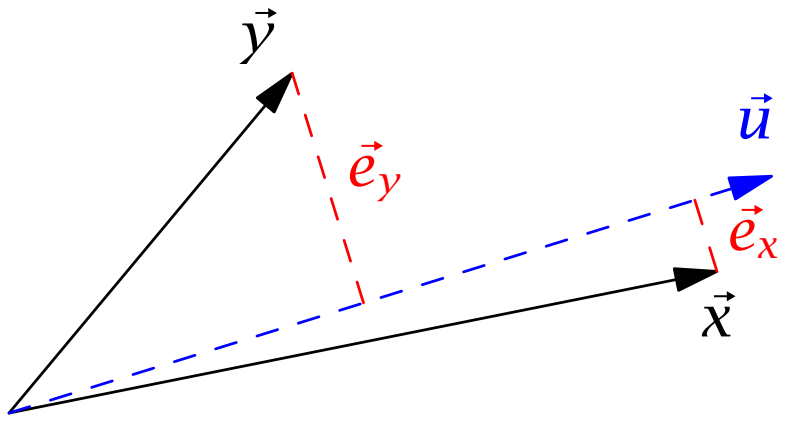




Vector Geometry of Major Axis Regression



(a) OLS



(b) Major Axis Regression

Figure: Vector geometry of ordinary least-squares and major axis regression.