Computational Methods
CMSC/AMSC/MAPL 460

Least squares method: linear regression

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Fitting data to a model

- Practical science involves lots of fitting of data to models
- Difference between fitting and interpolation?
  - Interpolation, the fit function passes through the point
  - Fitting, the fit function satisfies some error criterion
- Tasks arise commonly in science
  - Fit straight lines and curves to data
  - More generally fit data to a parametric model
- Parametric: Model contains parameters
  - Job of fitting is to estimate the parameters that "best" make the model fit the data
  - "best" → define best
- Simplest example of model fitting problem
  - Linear regression

Models

- Have a certain model structure
  - E.g., “linear” “quadratic” “trigonometric” “Gaussian”
- Models have specifiable parameters
- Model Structure Data Param.

Straight line: $a\,x + by + c = 0$ (x_i, y_i) a, b, c

Polynomial: $y = c_0 + c_1\,x + \ldots + c_n\,x^n$ (x_i, y_i) $c_0, c_1, \ldots, c_n$

- General model
- $y(x) \simeq \beta_1\,\phi_1(x) + \ldots + \beta_n\,\phi_n(x) +$
- E.g., $\simeq \beta_1\,x + \ldots + \beta_n\,\phi_n(x) +$
- Data (y_i, x_i) and
- $y = \Phi\beta$
- Solve $\beta = \Phi\backslash\mathbf{y}$

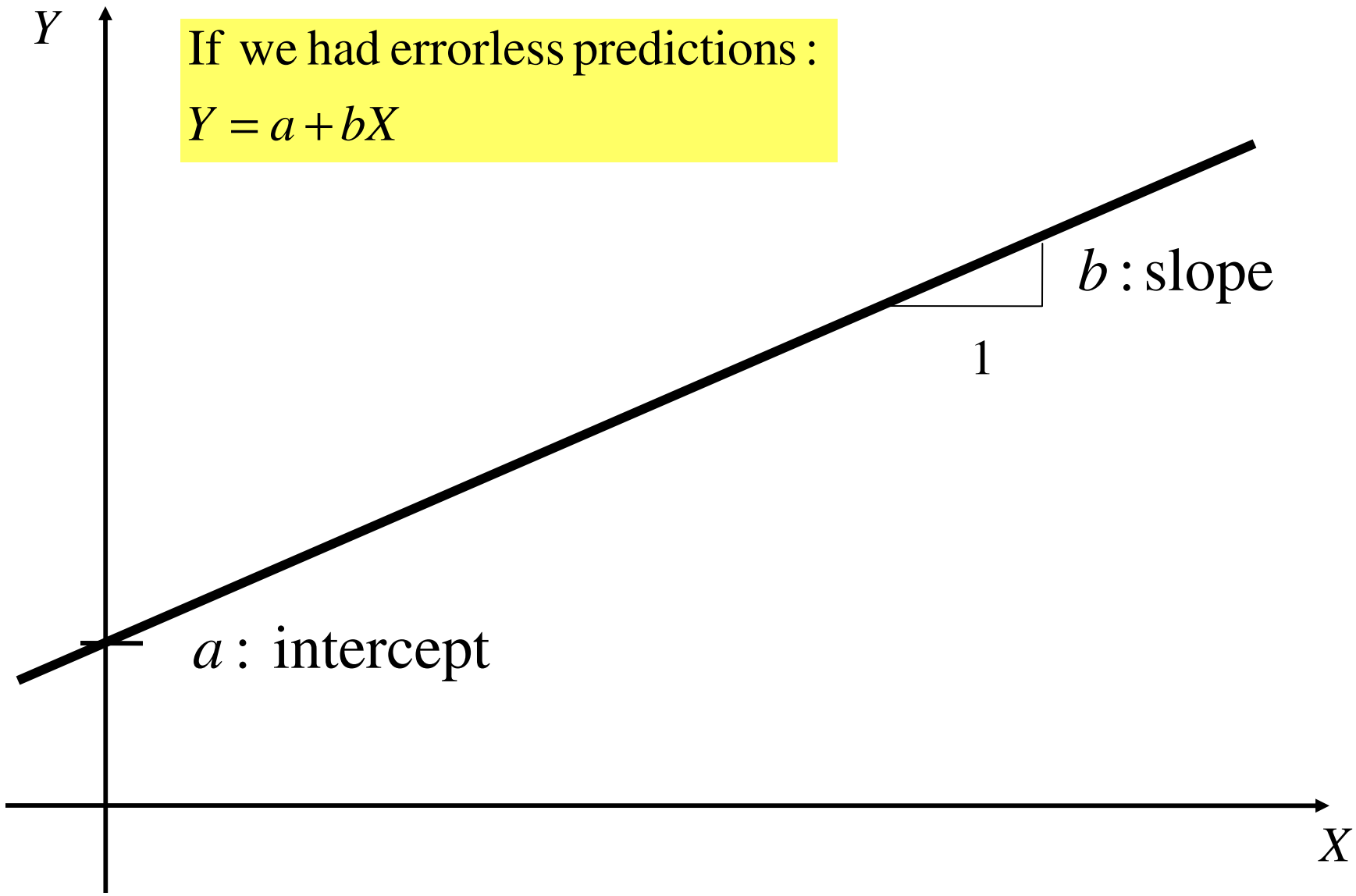
Relationships among Variables

- In much science we seek relations between variables

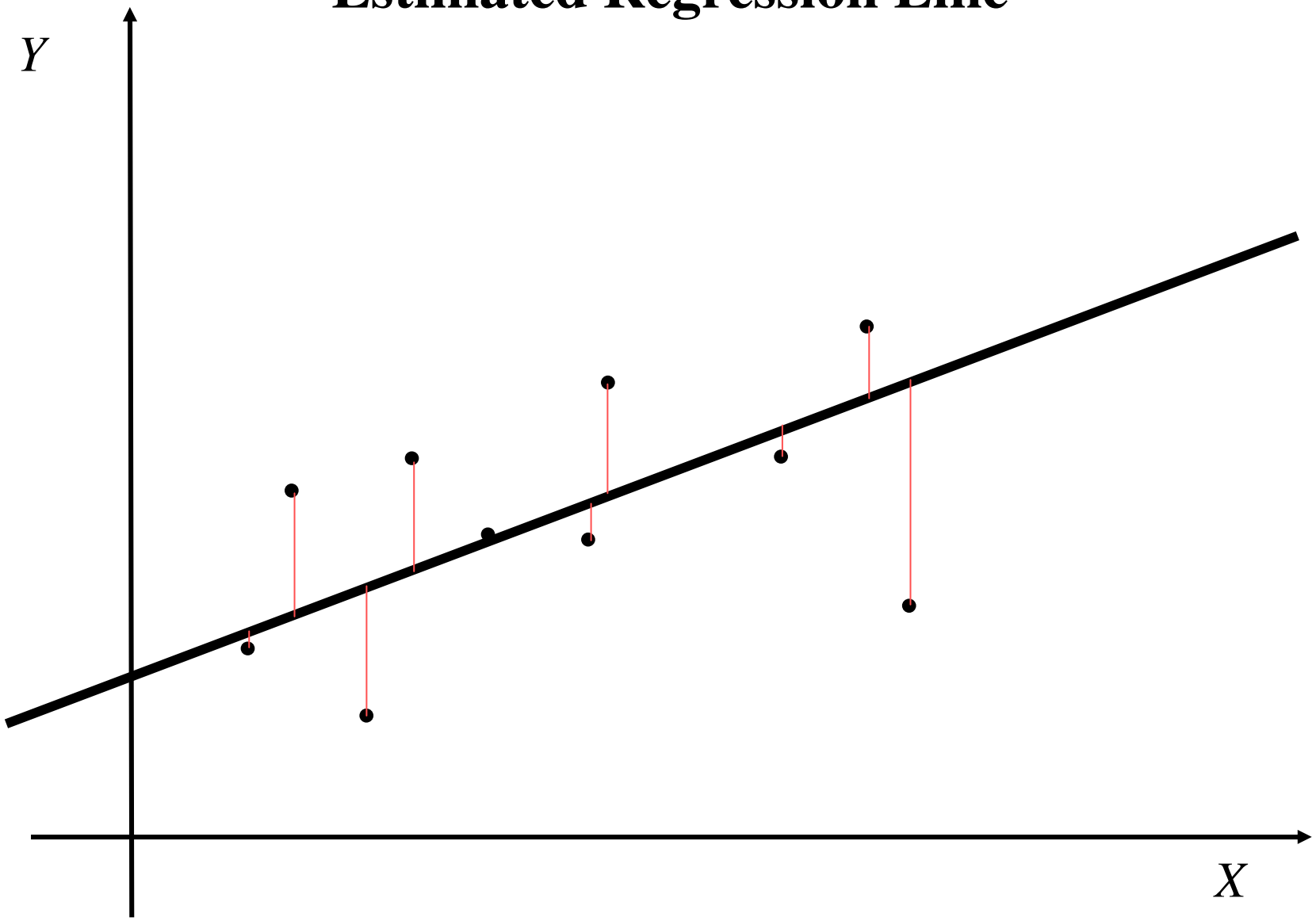
One variable is used to “explain” another variable

X Variable		Y Variable
Independent Variable	→	Dependent Variable
Explaining Variable		Response Variable
Exogenous Variable		Endogenous Variable
Predictor Variable		Criterion Variable

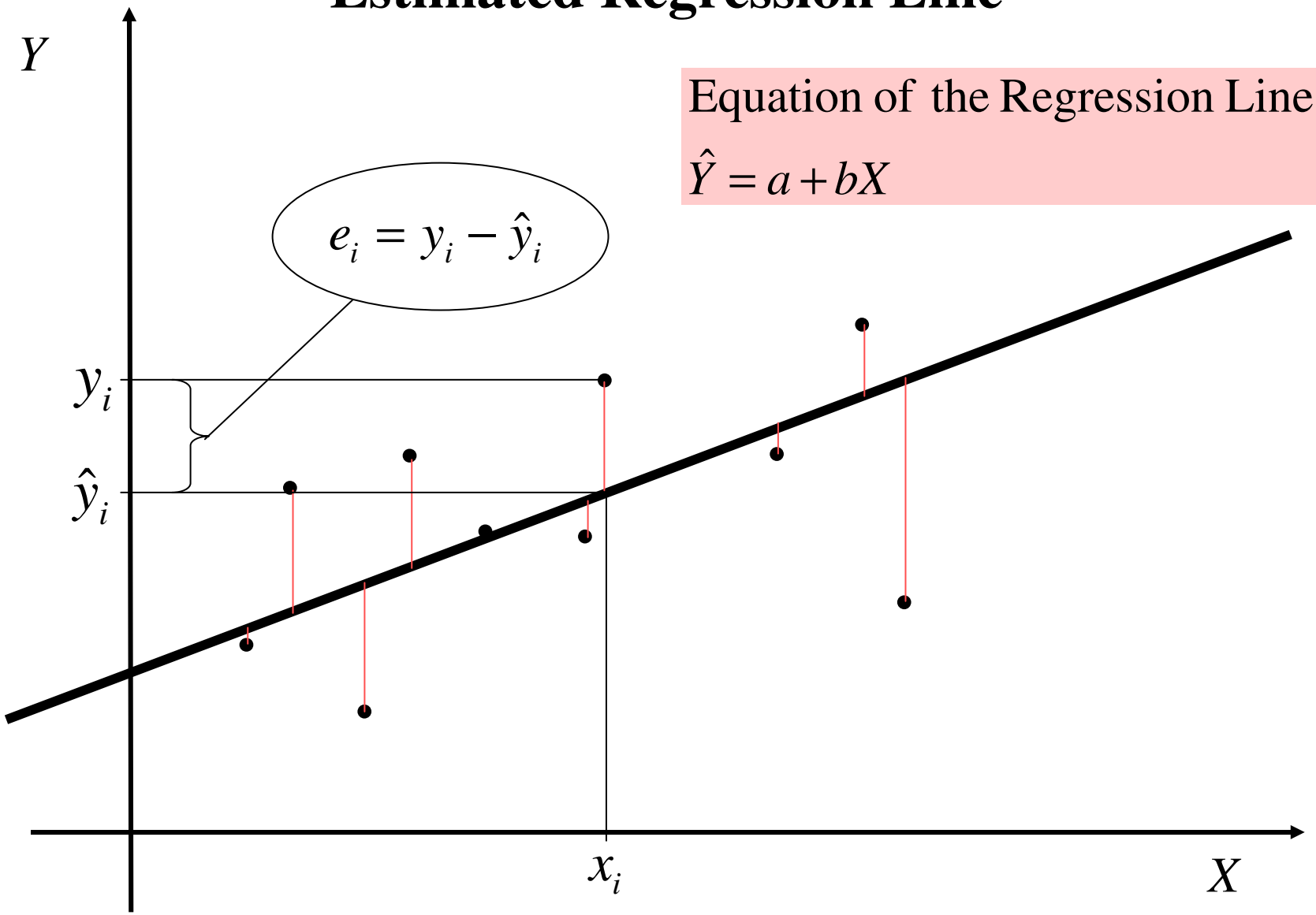
Simple Least-Squares Regression



Estimated Regression Line



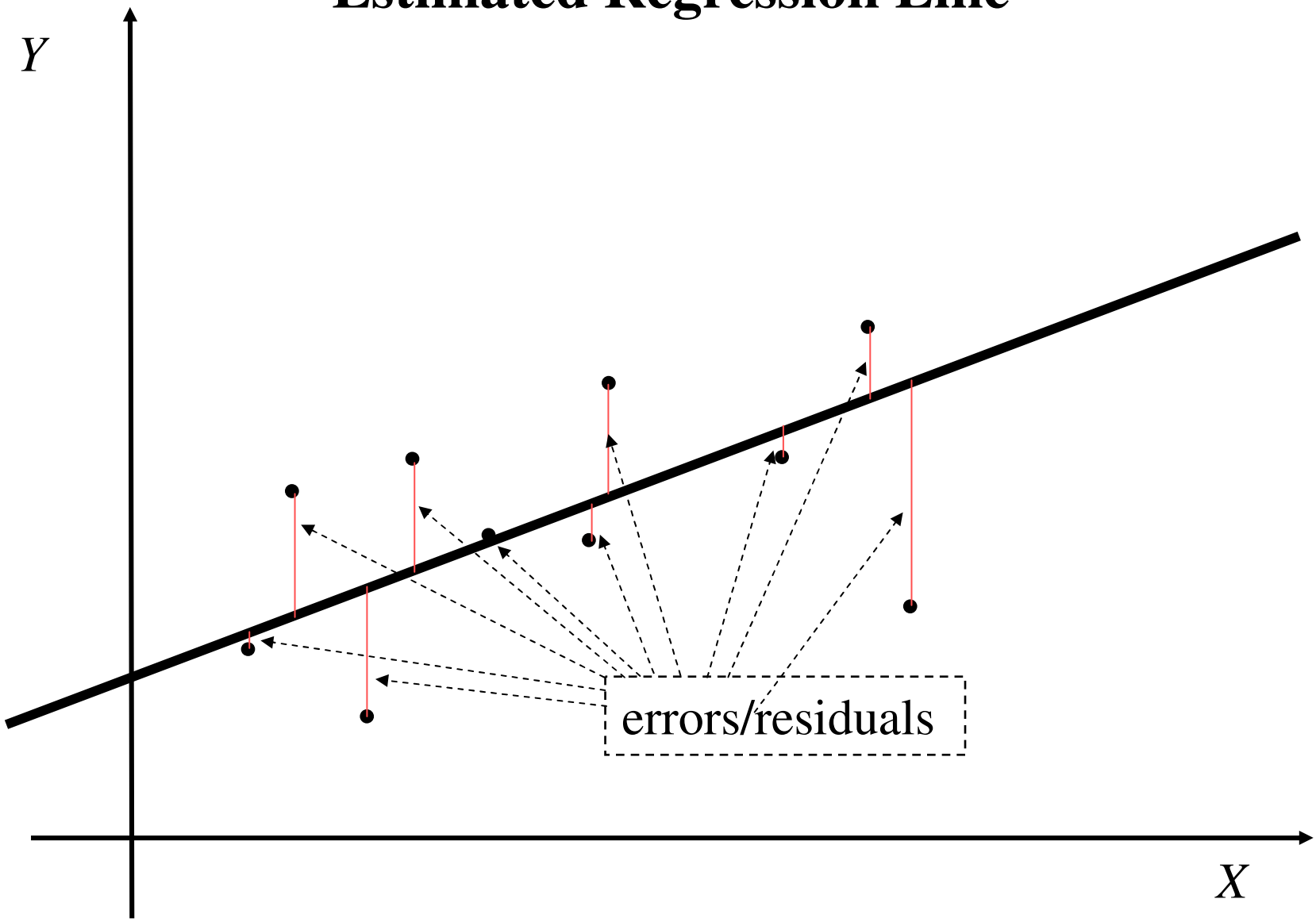
Estimated Regression Line



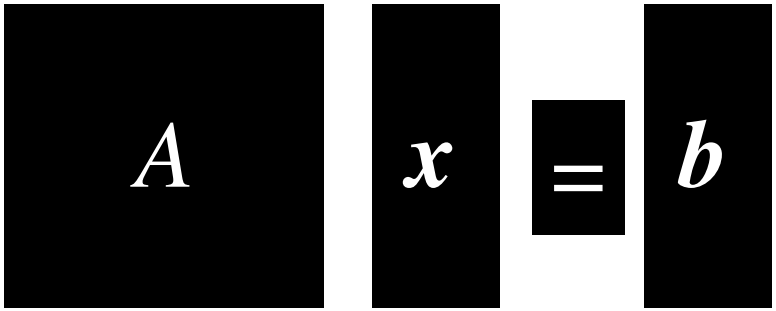
Equation of the Regression Line:

$\hat{Y} = a + bX$

Estimated Regression Line



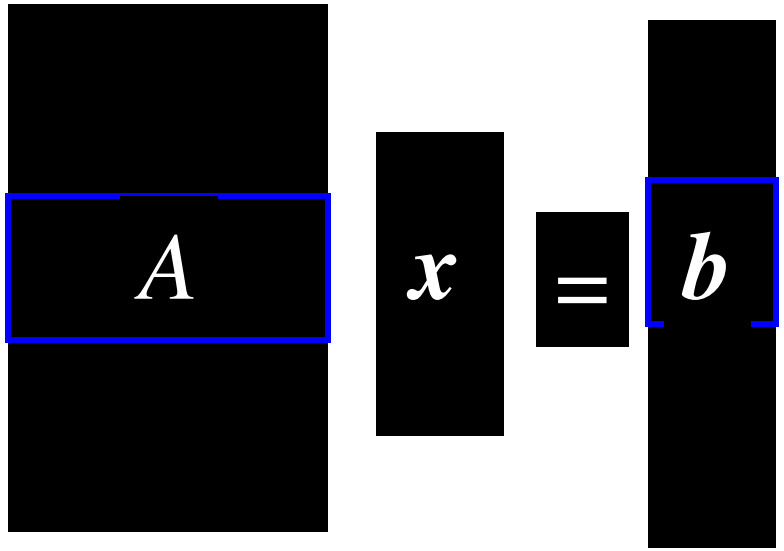
Linear Systems



Square system:

- unique solution
- Gaussian elimination

For straight line fitting we need to find two parameters.
However each of the data points provides an estimate of the error



Rectangular system ??

- underconstrained: infinity of solutions
- overconstrained: no solution

Minimize $|Ax-b|^2$

How do we find a and b?

In Least-Squares Regression:

Find a, b to minimize the sum of squared errors/residuals

$$\sum_{\mathrm{i}=1}^{\mathrm{N}} (e_i)^2 = \sum_{\mathrm{i}=1}^{\mathrm{N}} (y_i - [bx_i + a])^2$$

Least Squares for more complex models

- Number of equations and unknowns may not match
- Look for solution by minimizing some cost function
- Simplest and most intuitive cost function: $\|\mathbf{Ax} - \mathbf{b}\|_2$
- Define for each data point x_i a residual r_i
- *Minimize* $\sum_i r_i\, r_i$ with respect to x_l

  $\sum_i r_i\, r_i = \sum_j (A_{ij}x_j - b_i).\ \sum_k (A_{ik}x_k - b_i)$

$$\frac{\partial}{\partial x_l}(A_{ij}x_j - b_i)\bullet(A_{ik}x_k - b_i) = 0$$

$$(A_{ij}\delta_{jl})\bullet(A_{ik}x_k - b_i) + (A_{ij}x_j - b_i)\bullet(A_{ik}\delta_{kl}) = 0$$

$$A_{il}\bullet(A_{ik}x_k - b_i) + (A_{ij}x_j - b_i)\bullet A_{il} = 2\left(A_{il}A_{ik}x_k - A_{il}b_i\right) = 0$$

$$A_{il}A_{ik}x_k = A_{il}b_i$$

Other Norms

- Here we fit using the "least-squares" or L_2 norm
- Could minimize the residual in other norms
- For example we may have more confidence in some data, and want to be sure that their residual is lower
  - Attach a weight to each residual

$$\|r\|_w^2 = \sum_1^m w_i r_i^2$$

- Or we may like the 1-norm or infinity norm better

$$\|r\|_1 = \sum_1^m |r_i| \qquad \|r\|_\infty = \max_i |r_i|$$

Normal equations

- The system $A^t A x = A^t b$
  is called the Normal equations
- Can solve least squares problems using these
- For A size $m \times n$ and x of size n and b of size m what are the dimensions of the normal equations?
  - $n \times n$
- Solve via LU decomposition
- Is this a good idea?
  - Somewhat expensive as we have to form $A^t A$ which involves matrix multiplication and then solution
  - More importantly it is poorly conditioned
  - $\text{cond}(A^t A) = (\text{cond}(A))^2$