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.

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

Relationships among Variables

- In much science we seek relations between variables

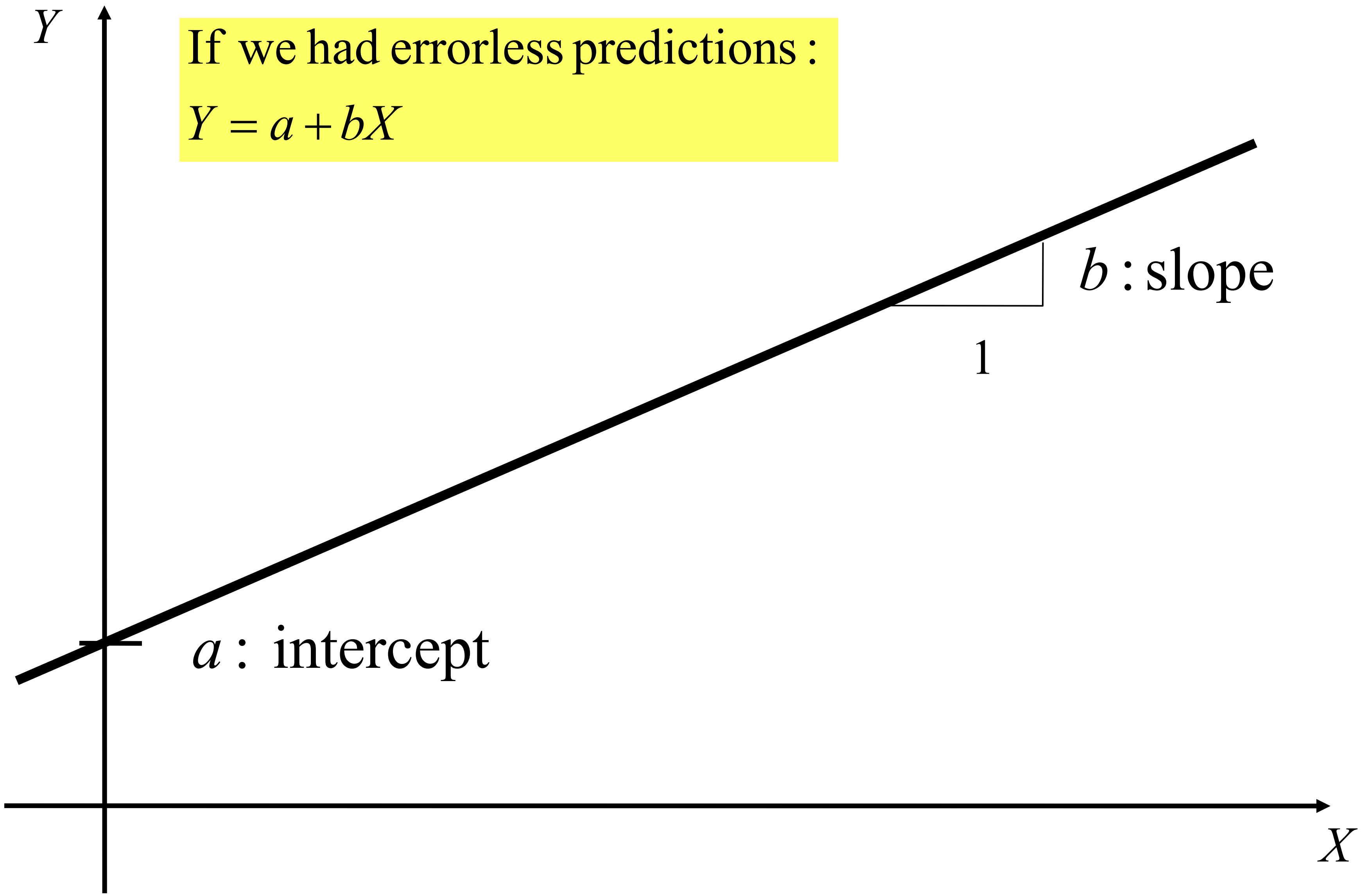
One variable is used to "explain" another variable

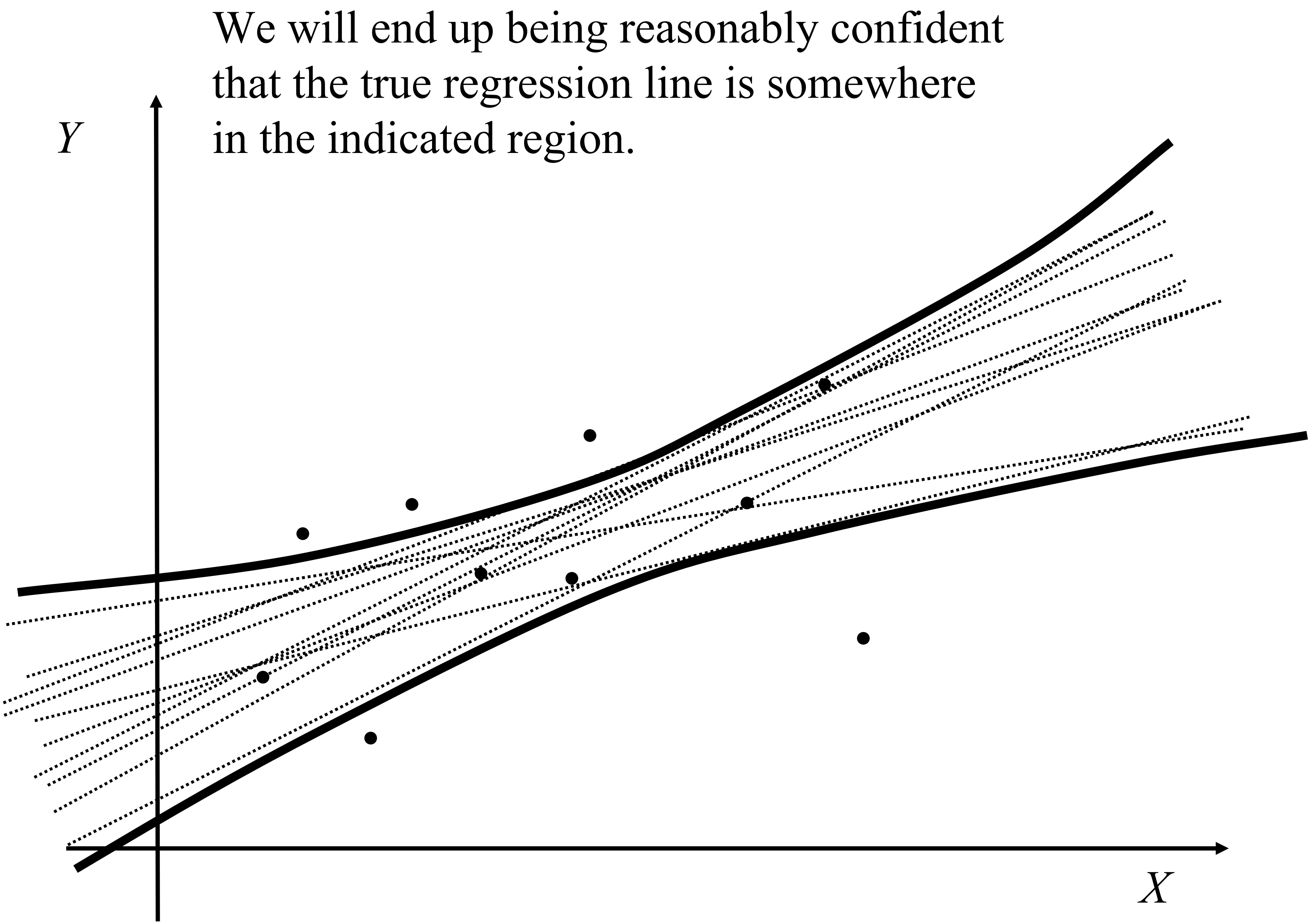
X Variable		Y Variable
Independent Variable	→	Dependent Variable
Explaining Variable		Response Variable
Exogenous Variable		Endogenous Variable
Predictor Variable		Criterion Variable

Simple Least-Squares Regression

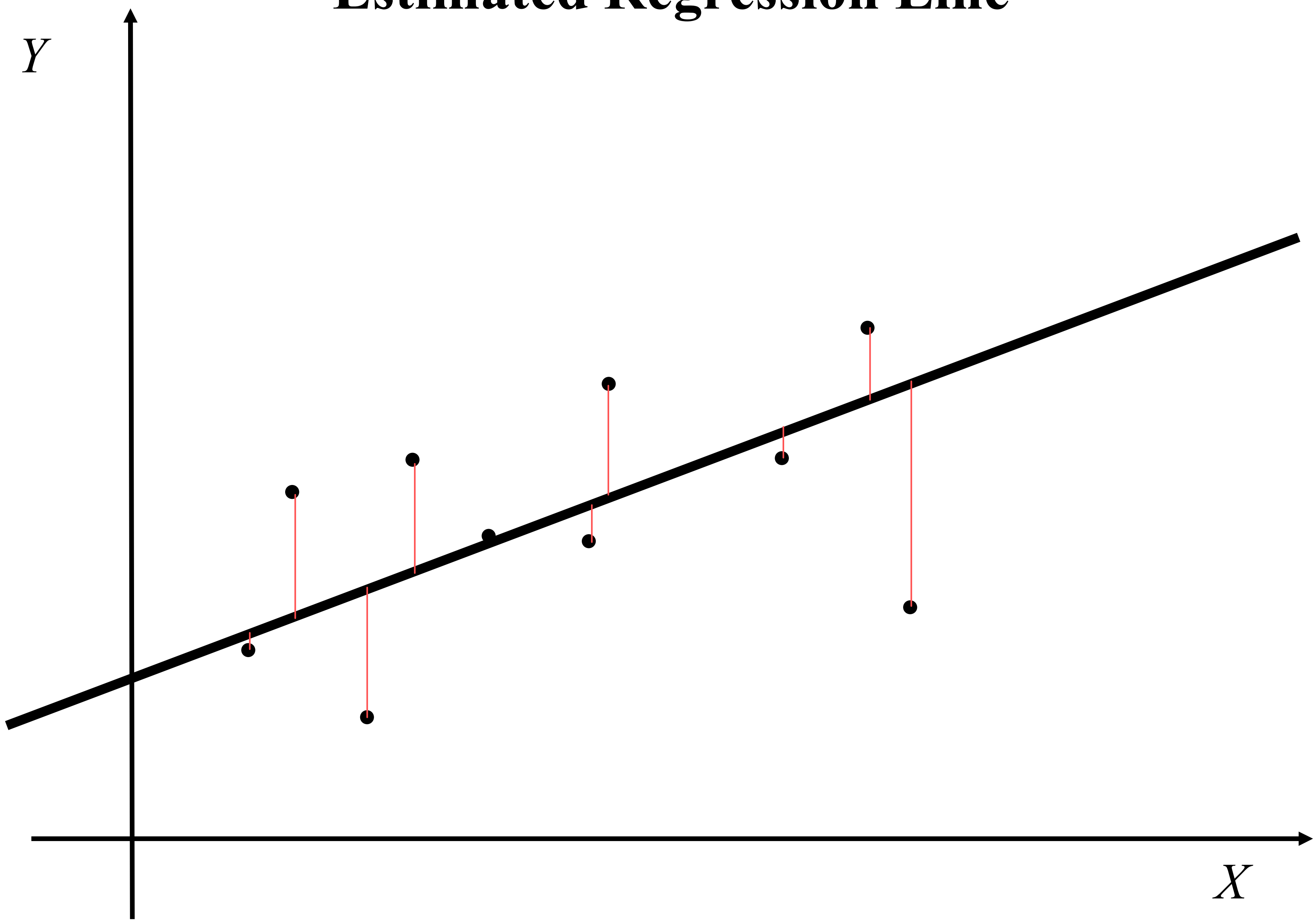
If we had errorless predictions :

$Y = a + bX$

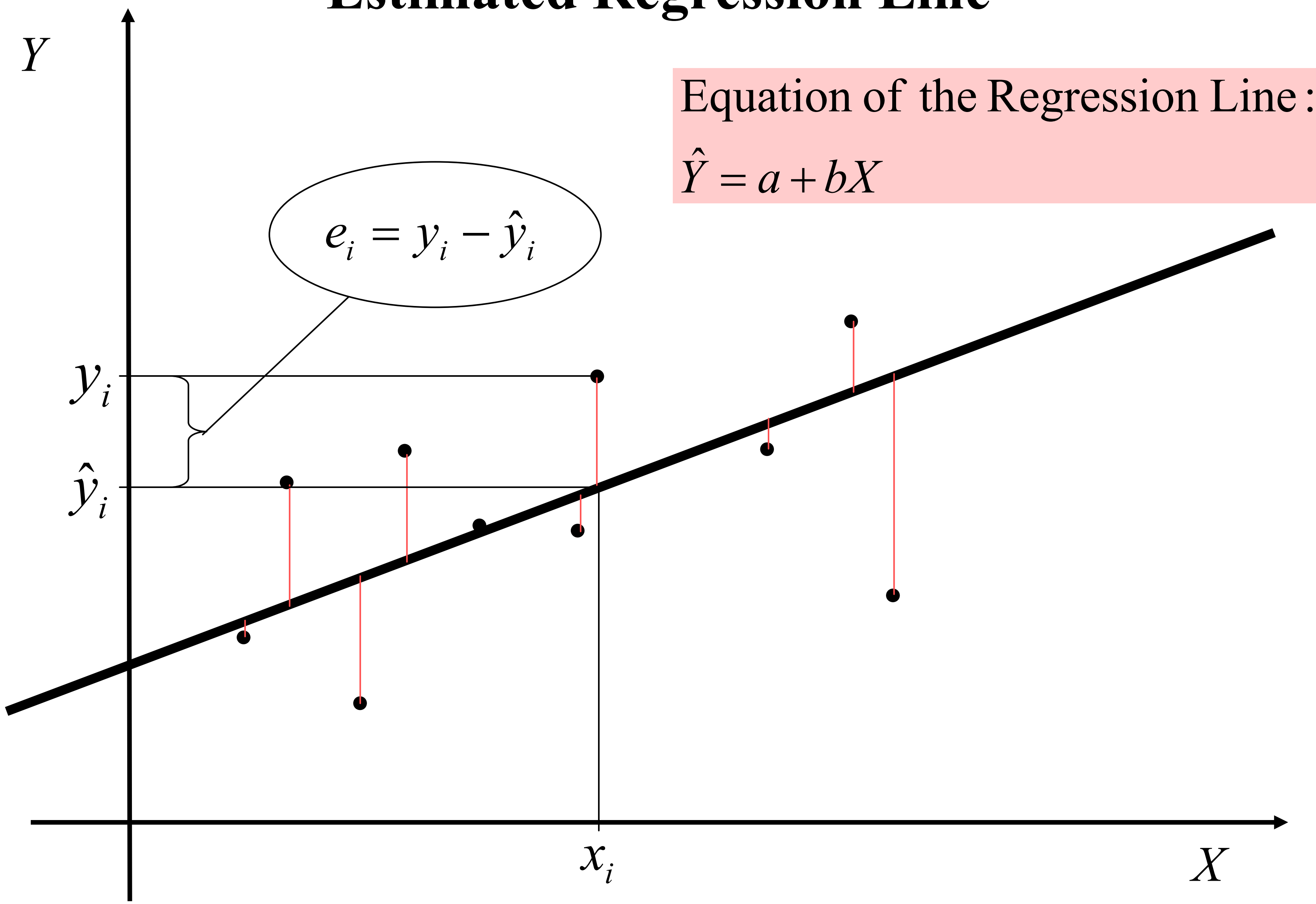



We will end up being reasonably confident that the true regression line is somewhere in the indicated region.
Y
X

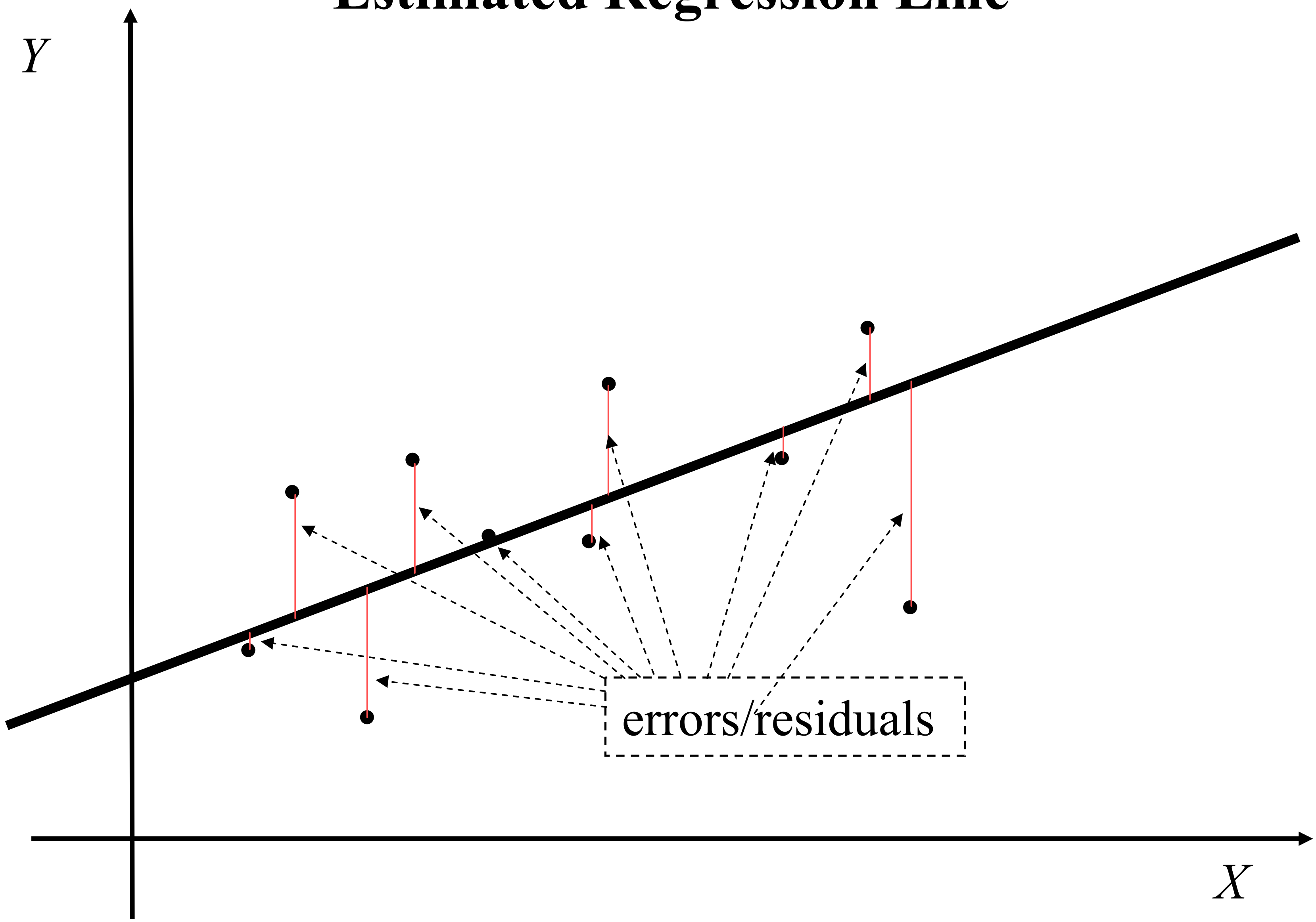
Estimated Regression Line



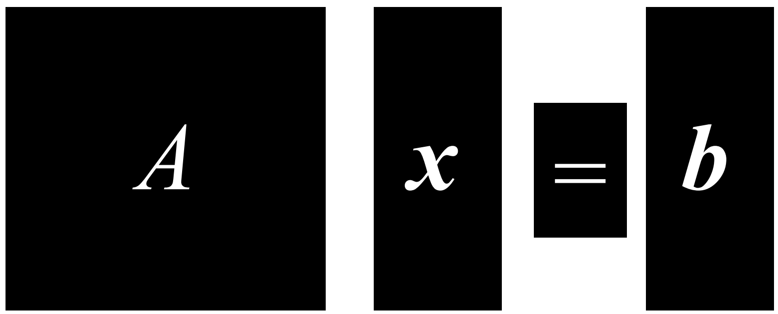
Estimated Regression Line



Estimated Regression Line



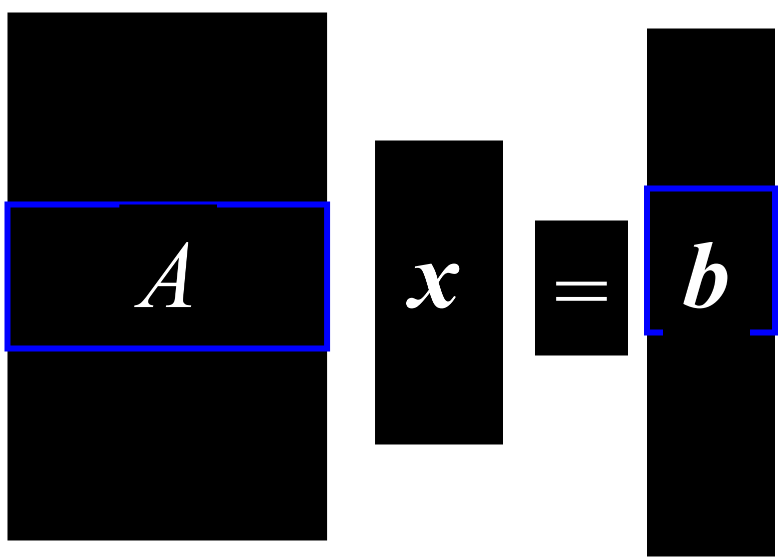
Linear Systems



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

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

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

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

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

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

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

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

In Least-Squares Regression:

$$b = \frac{\sum_{i=1}^{N}(X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^{N}(X_i - \overline{X})^2}, \qquad a = \overline{Y} - b\overline{X}$$

Computational Formula

$$b = \frac{N\sum_{i=1}^{N} X_i Y_i - \left(\sum_{i=1}^{N} X_i\right)\left(\sum_{i=1}^{N} Y_i\right)}{N\sum_{i=1}^{N} X_i^2 - \left(\sum_{i=1}^{N} X_i\right)^2}$$

Linear models

- Some models considered are "linear" or "separable"
  - (does not mean straight lines)
  - Means that we can separate the "structure" and "parameters" as a matrix-vector product
  - "structure" forms a matrix and "parameters" a vector
- Goal of model fitting: find the parameters
- Question: Is the Gaussian model a linear one?
  - Can be made separable by taking logs

$$y(t) \approx K e^{\lambda t}$$

$$\log y \approx \beta_1 t + \beta_2, \text{ with } \beta_1 = \lambda, \; \beta_2 = \log K$$

  - However if there are sums of gaussians or exponentials the model is not separable

$$y(t) \approx \beta_1 e^{-\left(\frac{t-\mu_1}{\sigma_1}\right)^2} + \dots \beta_n e^{-\left(\frac{t-\mu_n}{\sigma_n}\right)^2}$$

Models

- Have a certain model structure
  - E.g., " straight line" "parabolic" "trigonometric" "Gaussian"
- Models have specifiable parameters
- e.g.
- Model Structure Data Parameters

Model	Structure	Data	Parameters
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)	$(c_0, c_1, \ldots, c_n)$
Trig.:	$y = c_0 + c_1 \sin x + \ldots + c_n \sin nx$	(x_i, y_i)	$(c_0, c_1, \ldots, c_n)$
Gaussian	$y = c_0 \exp(-(x-\mu)^2/\sigma^2)$	(x_i, y_i)	(c_0, σ, μ)
"Kernel/RBF"	$y = \sum_i a_i k(x, x_i)$	(x_i, y_i)	(a_i) and (x_i)

- These models are all separable

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
  - $\mathrm{cond}(A^t A) = (\mathrm{cond}(A))^2$