Data Modeling and Least Squares Fitting 2

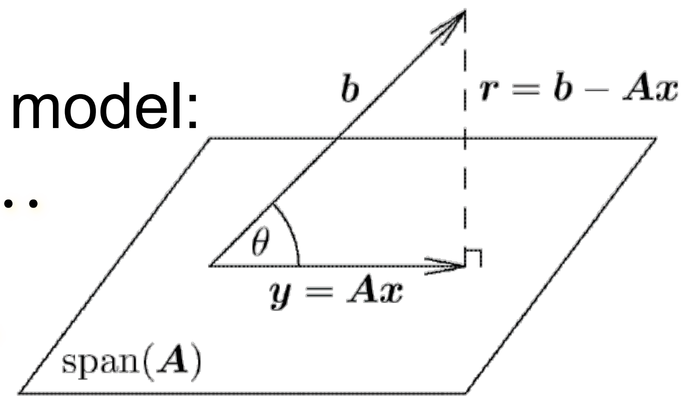
COS 323

Last time

- Data modeling
- Motivation of least-squares error
- Formulation of linear least-squares model:

$$y_i = a\,f(\vec{x}_i) + b\,g(\vec{x}_i) + c\,h(\vec{x}_i) + \cdots$$

Given $(\vec{x}_i, y_i)$, solve for $a, b, c, \ldots$



- Solving using ormal equations (bad), pseudoinverse
- Illustrating least-squares with special cases: constant, line
- Weighted least squares
- Evaluating model quality

Today

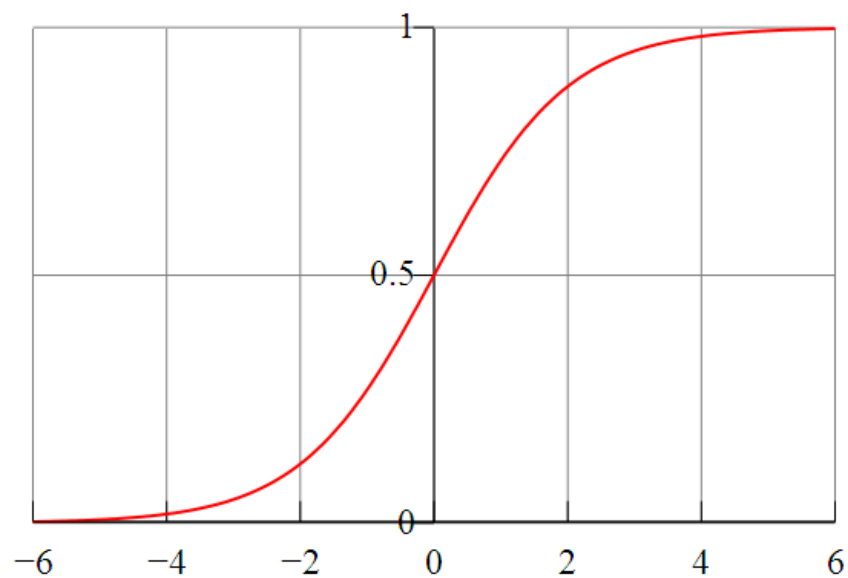
- Solving **non-linear** least squares
  - Newton, Gauss-Newton methods
  - Logistic regression and Levenberg-Marquardt method
- Dealing with outliers and bad data:
  Robust regression with M-Estimators
- Practical considerations
  - Is least squares an appropriate method for my data?
- Solving with Excel and Matlab

Example: Logistic Regression

- Model probability of an event based on values of explanatory variables, using generalized linear model, logistic function g(z)

$$p(\vec{x}) = g(ax_1 + bx_2 + \cdots)$$

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



Logistic Regression

- Assumes positive and negative examples are normally distributed, with different means but same variance
- Applications: predict odds of election victories, sports events, medical outcomes, etc.

Nonlinear Least Squares

- Some problems can be rewritten to linear

$$y = ae^{bx}$$

$$\Rightarrow \quad (\log y) = (\log a) + bx$$

- Fit data points $(x_i, \log y_i)$ to $a^* + bx$, $a = e^{a^*}$
- Big problem: this no longer minimizes squared error!

Nonlinear Least Squares

- Can write error function, minimize directly

$$\chi^2 = \sum_i \left(y_i - f(x_i, a, b, \ldots)\right)^2$$

$$\text{Set } \frac{\partial}{\partial a} = 0, \frac{\partial}{\partial b} = 0, \text{etc.}$$

- For the exponential, no analytic solution for a, b:

$$\chi^2 = \sum_i \left(y_i - ae^{bx_i}\right)^2$$

$$\frac{\partial}{\partial a} = \sum_i -2e^{bx_i}\left(y_i - ae^{bx_i}\right) = 0$$

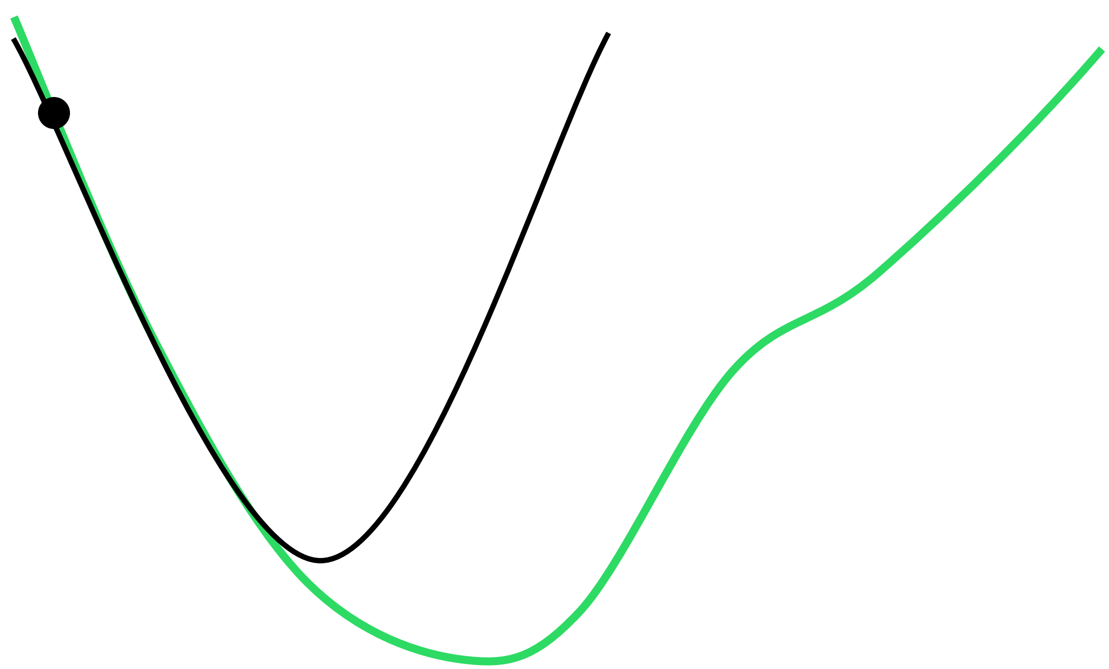
$$\frac{\partial}{\partial b} = \sum_i -2ax_ie^{bx_i}\left(y_i - ae^{bx_i}\right) = 0$$

Newton's Method

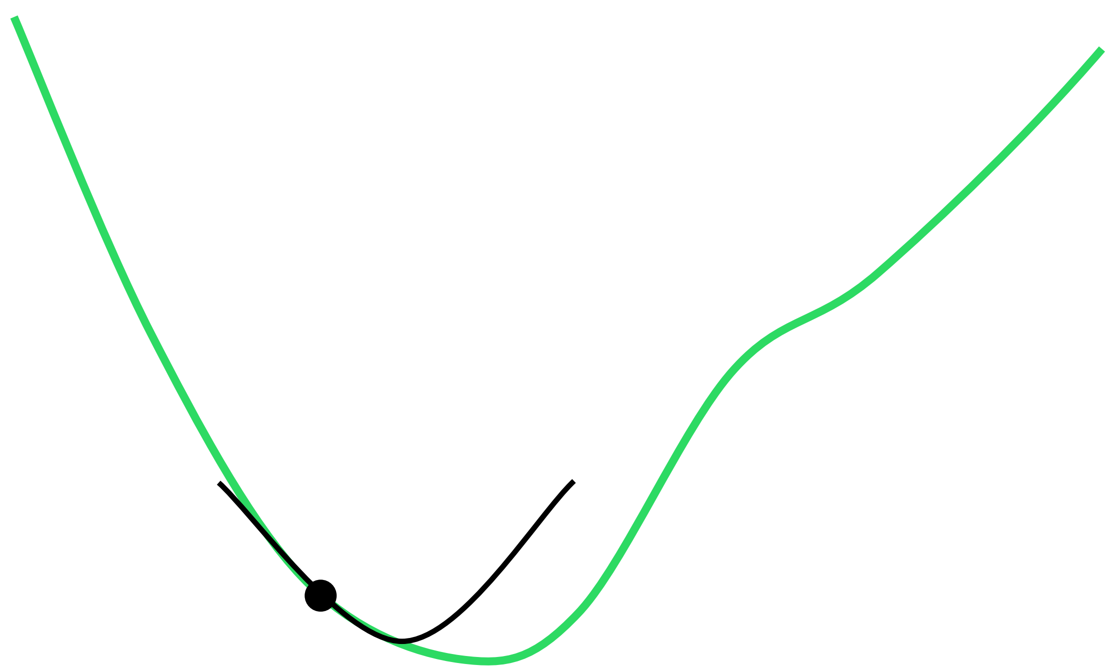
- Apply Newton's method for minimization:
  - 1-dimensional: $$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$
  - n-dimensional: $$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_i - H^{-1}G$$

where H is Hessian (matrix of all 2nd derivatives) and G is gradient (vector of all 1st derivatives)

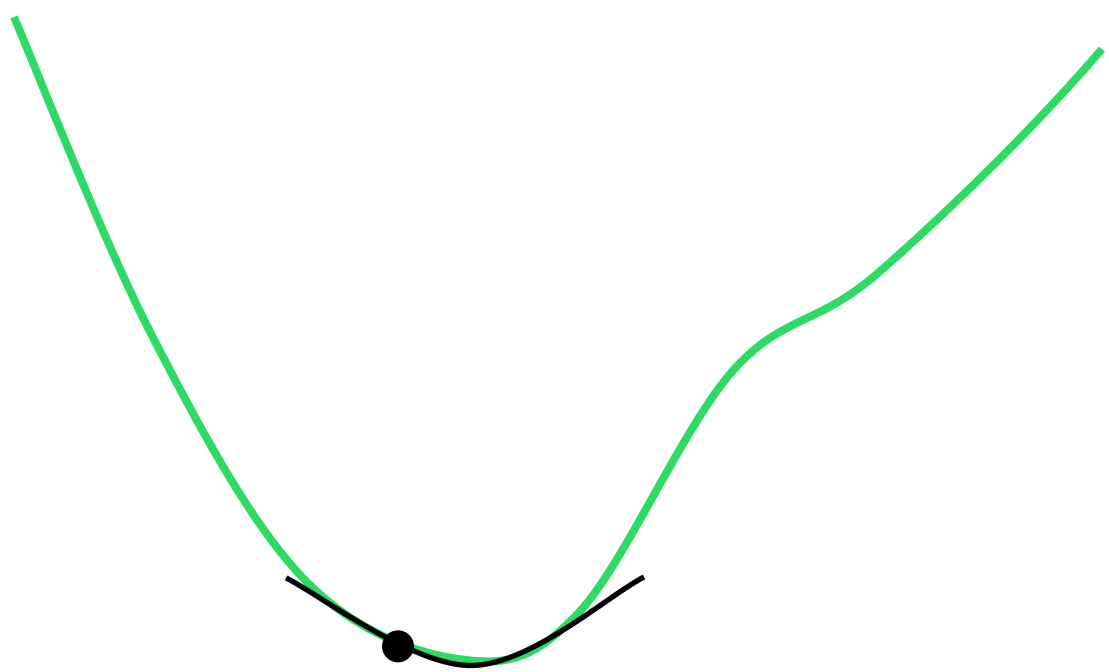
Newton's Method



Newton's Method



Newton's Method



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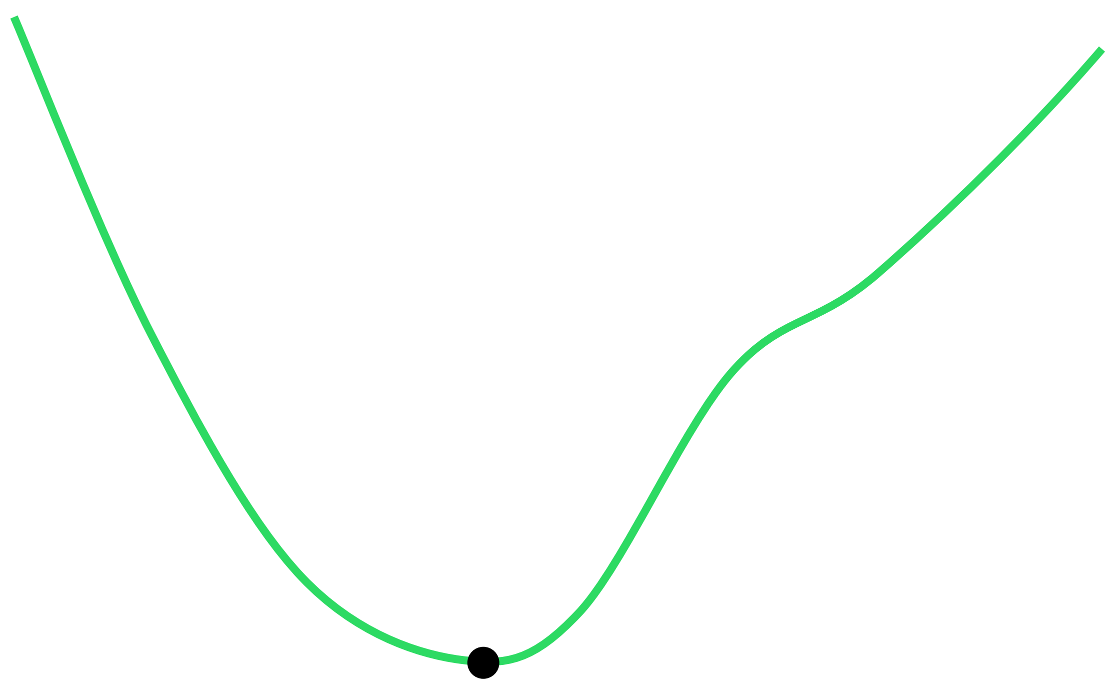

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Newton's Method for Least Squares

$$\chi^2(a,b,\ldots) = \sum_i \left(y_i - f(x_i,a,b,\ldots)\right)^2$$

$$G = \begin{bmatrix} \frac{\partial(\chi^2)}{\partial a} \\ \frac{\partial(\chi^2)}{\partial b} \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_i -2\frac{\partial f}{\partial a}\left(y_i - f(x_i,a,b,\ldots)\right) \\ \sum_i -2\frac{\partial f}{\partial b}\left(y_i - f(x_i,a,b,\ldots)\right) \\ \vdots \end{bmatrix}$$

$$H = \begin{bmatrix} \frac{\partial^2(\chi^2)}{\partial a^2} & \frac{\partial^2(\chi^2)}{\partial a \partial b} & \cdots \\ \frac{\partial^2(\chi^2)}{\partial a \partial b} & \frac{\partial^2(\chi^2)}{\partial b^2} & \cdots \\ & \vdots & \end{bmatrix}$$

- Gradient has 1st derivatives of *f*, Hessian 2nd

Gauss-Newton Iteration

- Consider 1 term of Hessian:

$$\frac{\partial^2(\chi^2)}{\partial a^2} = \frac{\partial}{\partial a}\left(\sum_i -2\tfrac{\partial f}{\partial a}\big(y_i - f(x_i,a,b,\ldots)\big)\right)$$

$$= -2\sum_i \tfrac{\partial^2 f}{\partial a^2}\cancel{\big(y_i - f(x_i,a,b,\ldots)\big)} + 2\sum_i \tfrac{\partial f}{\partial a}\tfrac{\partial f}{\partial a}$$

- Equivalently, the book version:

$$s_k = \left(\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k) + \cancel{\sum_{i=1}^{m} r_i(\mathbf{x}_k)\mathbf{H}_{r_i}(\mathbf{x}_k)}\right)^{-1}\left(-\mathbf{J}^T(\mathbf{x}_k)r(\mathbf{x}_k)\right)$$

- If close to answer, residual is close to 0

Gauss-Newton Iteration

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} + s_i$$

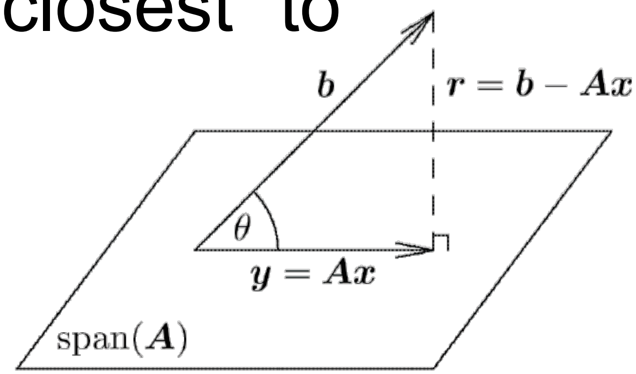
$s_i = -\mathbf{H}^{-1}\mathbf{G}$ (Newton) becomes

$$\underbrace{\underbrace{\mathbf{J}_i^{\mathrm{T}}\mathbf{J}_i}_{\text{estimate of Hessian}} s_i = \underbrace{\mathbf{J}_i^{\mathrm{T}} r_i}_{\text{gradient of residual}}}_{\text{solve this for } s_i}$$

$$J = \begin{pmatrix} \frac{\partial f}{\partial a}(x_1) & \frac{\partial f}{\partial b}(x_1) & \cdots \\ \frac{\partial f}{\partial a}(x_2) & \frac{\partial f}{\partial b}(x_2) & \\ \vdots & & \ddots \end{pmatrix}, \quad r = \begin{pmatrix} y_1 - f(x_1, a, b, \cdots) \\ y_2 - f(x_2, a, b, \cdots) \\ \vdots \end{pmatrix}$$

Last week: Linear Least Squares Solution

- Interpretation: find x that comes "closest" to satisfying Ax=b
  - i.e., minimize b–Ax
  - i.e., minimize || b–Ax ||
  - Equivalently, find x such that r is orthogonal to span(A)



$$0 = \mathbf{A}^T\mathbf{r} = \mathbf{A}^T(\mathbf{b} - \mathbf{A}\mathbf{x})$$

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$$

Gauss-Newton Iteration

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estimate of Hessian $\underbrace{\mathbf{J}_i^{\mathrm{T}}\mathbf{J}_i s_i = \mathbf{J}_i^{\mathrm{T}} r_i}_{\text{solve this for } s_i}$ gradient of residual

$$J = \begin{pmatrix} \frac{\partial f}{\partial a}(x_1) & \frac{\partial f}{\partial b}(x_1) & \cdots \\ \frac{\partial f}{\partial a}(x_2) & \frac{\partial f}{\partial b}(x_2) & \\ \vdots & & \ddots \end{pmatrix}, \quad r = \begin{pmatrix} y_1 - f(x_1, a, b, \cdots) \\ y_2 - f(x_2, a, b, \cdots) \\ \vdots \end{pmatrix}$$

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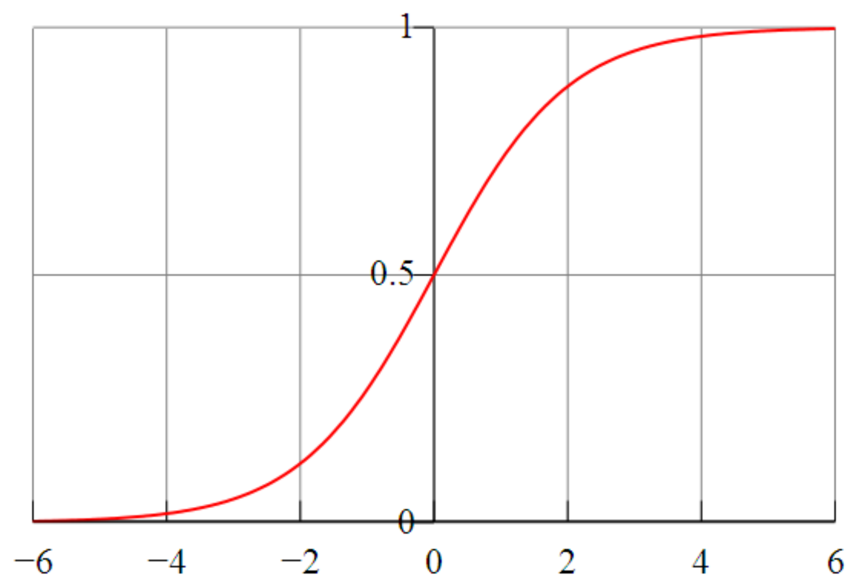


Logistic Regression

- Assumes positive and negative examples are normally distributed, with different means but same variance
- Applications: predict odds of election victories, sports events, medical outcomes, etc.
- Estimate parameters a, b, … using Gauss-Newton on individual positive, negative examples
- Handy hint: $g'(z) = g(z)\,(1-g(z))$

Gauss-Newton++:
The Levenberg-Marquardt Algorithm

Levenberg-Marquardt

- Newton (and Gauss-Newton) work well when close to answer, terribly when far away
- Steepest descent safe when far away
- Levenberg-Marquardt idea: let's do both

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} - \alpha G - \beta \begin{pmatrix} \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial a} & \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \cdots \\ \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \sum \frac{\partial f}{\partial b}\frac{\partial f}{\partial b} & \cdots \\ & \vdots & \end{pmatrix}^{-1} G$$

Steepest descent

Gauss-Newton

Levenberg-Marquardt

- Trade off between constants depending on how far away you are…
- Clever way of doing this:

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} - \begin{pmatrix} (1+\lambda)\Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial a} & \Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \cdots \\ \Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & (1+\lambda)\Sigma \frac{\partial f}{\partial b}\frac{\partial f}{\partial b} & \cdots \\ & \vdots & \end{pmatrix}^{-1} G$$

- If λ is small, mostly like Gauss-Newton
- If λ is big, matrix becomes mostly diagonal, behaves like steepest descent

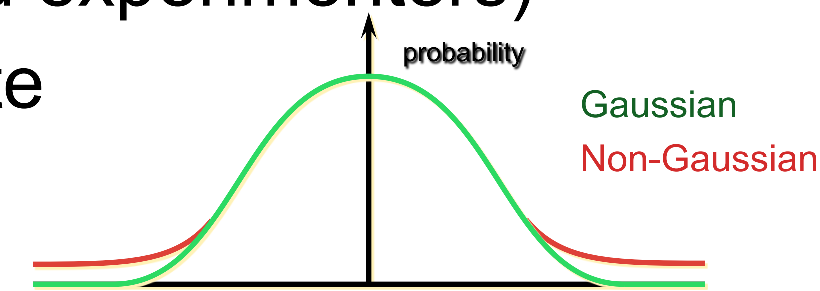
Levenberg-Marquardt

- Final bit of cleverness: adjust λ depending on how well we're doing
  - Start with some λ, e.g. 0.001
  - If last iteration *decreased* error, *accept* the step and *decrease* λ to $\lambda/10$
  - If last iteration *increased* error, *reject* the step and *increase* λ to 10λ
- Result: fairly stable algorithm, not too painful (no 2nd derivatives), used a lot

Dealing with Outliers

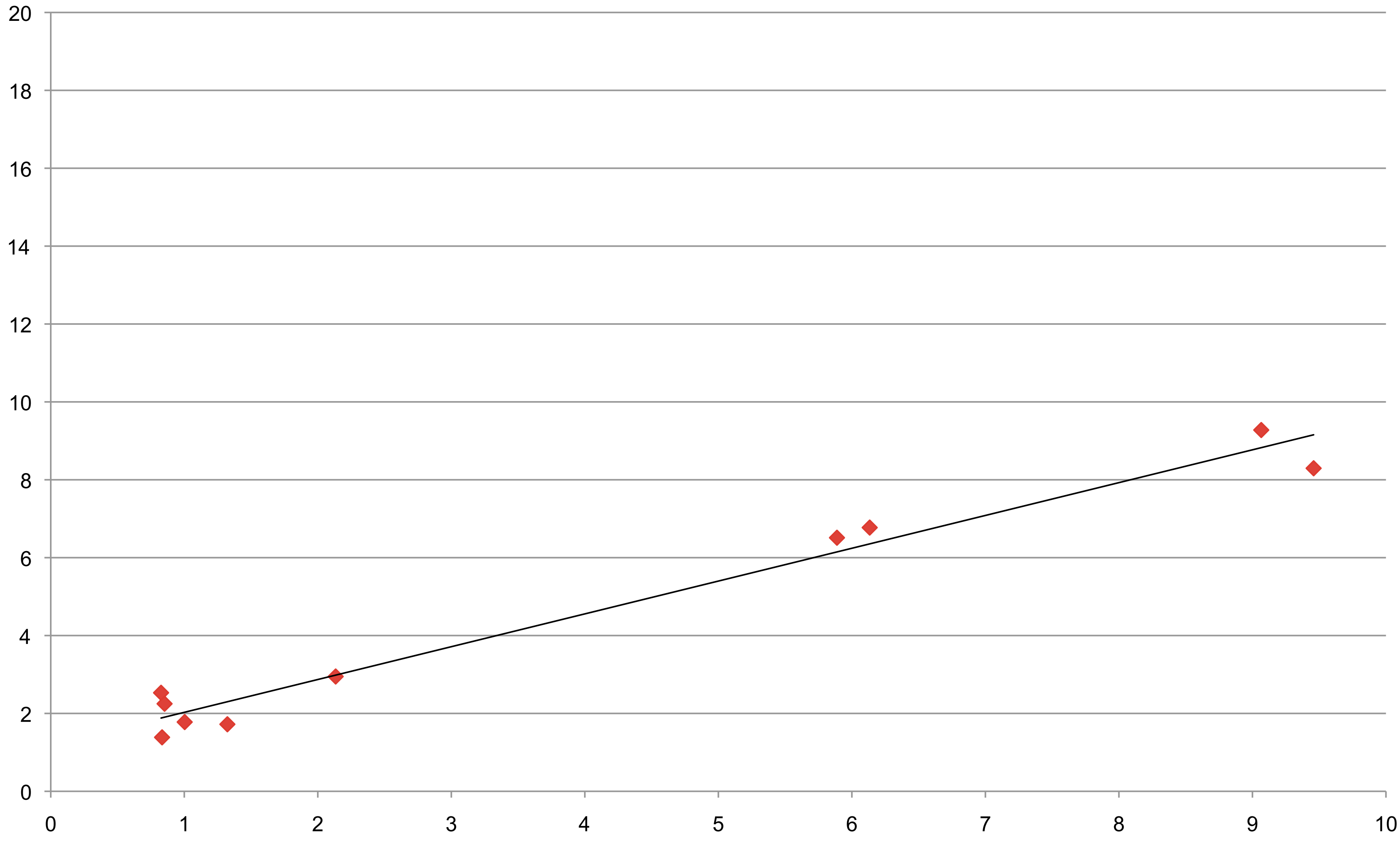
Outliers

- A lot of derivations assume Gaussian distribution for errors
- Unfortunately, nature (and experimenters) sometimes don't cooperate

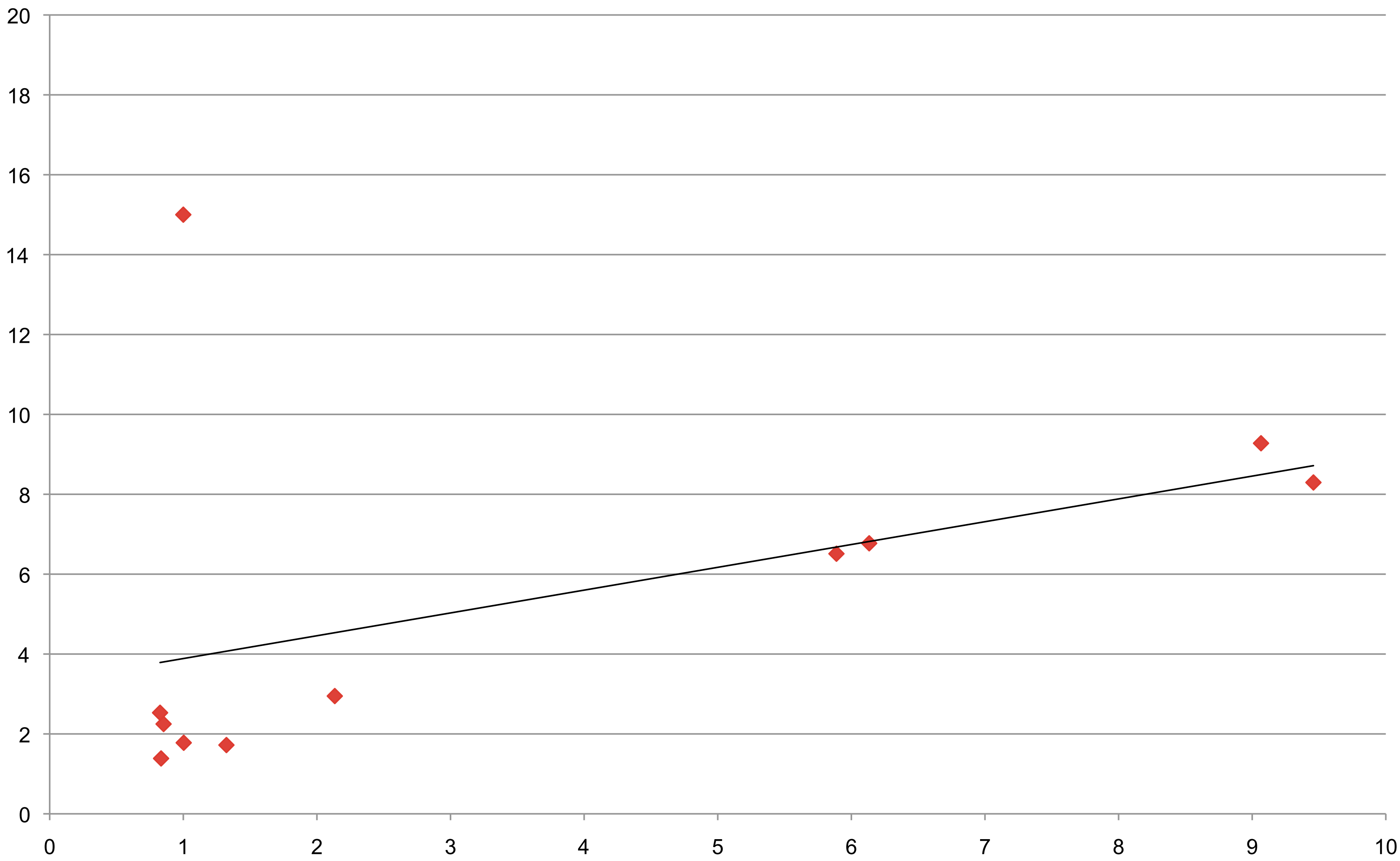


- Outliers: points with extremely low probability of occurrence (according to Gaussian statistics)
- Can have strong influence on least squares

Example: without outlier



Example: with outlier



Robust Estimation

- Goal: develop parameter estimation methods insensitive to *small* numbers of *large* errors
- General approach: try to give large deviations less weight
- e.g., **Median** is a robust measure, **mean** is not
- **M-estimators: minimize some function other than square of y – f(x,a,b,…)**

Least Absolute Value Fitting

- Minimize $\sum_i \left| y_i - f(x_i, a, b, \ldots) \right|$
  instead of $\sum_i \left(y_i - f(x_i, a, b, \ldots) \right)^2$

- Points far away from trend get comparatively less influence

Example: Constant

- For constant function $y = a$, minimizing $\Sigma(y-a)^2$ gave a = mean
- Minimizing $\Sigma|y-a|$ gives a = median

Least Squares vs. Least Absolute Deviations

- LS:
  - Not robust
  - Stable, unique solution
  - Solve with normal equations, Gauss-Newton, etc.
- LAD
  - Robust
  - Unstable, not necessarily unique
  - Requires iterative solution method (e.g. simplex)
- Interactive applet: http://www.math.wpi.edu/Course_Materials/SAS/lablets/7.3/7.3c/lab73c.html

Doing Robust Fitting

- In general case, nasty function: discontinuous derivative
- Simplex method often a good choice

Iteratively Reweighted Least Squares

- Sometimes-used approximation:
  convert to iteratively weighted least squares

$$\sum_i \left| y_i - f(x_i, a, b, \ldots) \right|$$

$$= \sum_i \frac{1}{\left| y_i - f(x_i, a, b, \ldots) \right|} \left(y_i - f(x_i, a, b, \ldots) \right)^2$$

$$= \sum_i w_i \left(y_i - f(x_i, a, b, \ldots) \right)^2$$

with w_i based on previous iteration

Review: Weighted Least Squares

- Define weight matrix W as

$$\mathbf{W} = \begin{pmatrix} w_1 & & & & 0 \\ & w_2 & & & \\ & & w_3 & & \\ & & & w_4 & \\ 0 & & & & \ddots \end{pmatrix}$$

- Then solve weighted least squares via

$$\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{A}\,x = \mathbf{A}^{\mathrm{T}}\mathbf{W}\,b$$

M-Estimators

Different options for weights

- Give even less weight to outliers

$$w_i = \frac{1}{\left|y_i - f(x_i, a, b, \ldots)\right|}$$ L$_1$

$$w_i = \frac{1}{\varepsilon + \left|y_i - f(x_i, a, b, \ldots)\right|}$$ "Fair"

$$w_i = \frac{1}{\varepsilon + \left(y_i - f(x_i, a, b, \ldots)\right)^2}$$ Cauchy / Lorentzian

$$w_i = e^{-k\left(y_i - f(x_i, a, b, \ldots)\right)^2}$$ Welsch

Iteratively Reweighted Least Squares

- Danger! This is not guaranteed to converge to the right answer!
  - Needs good starting point, which is available if initial least squares estimator is reasonable
  - In general, works OK if few outliers, not too far off

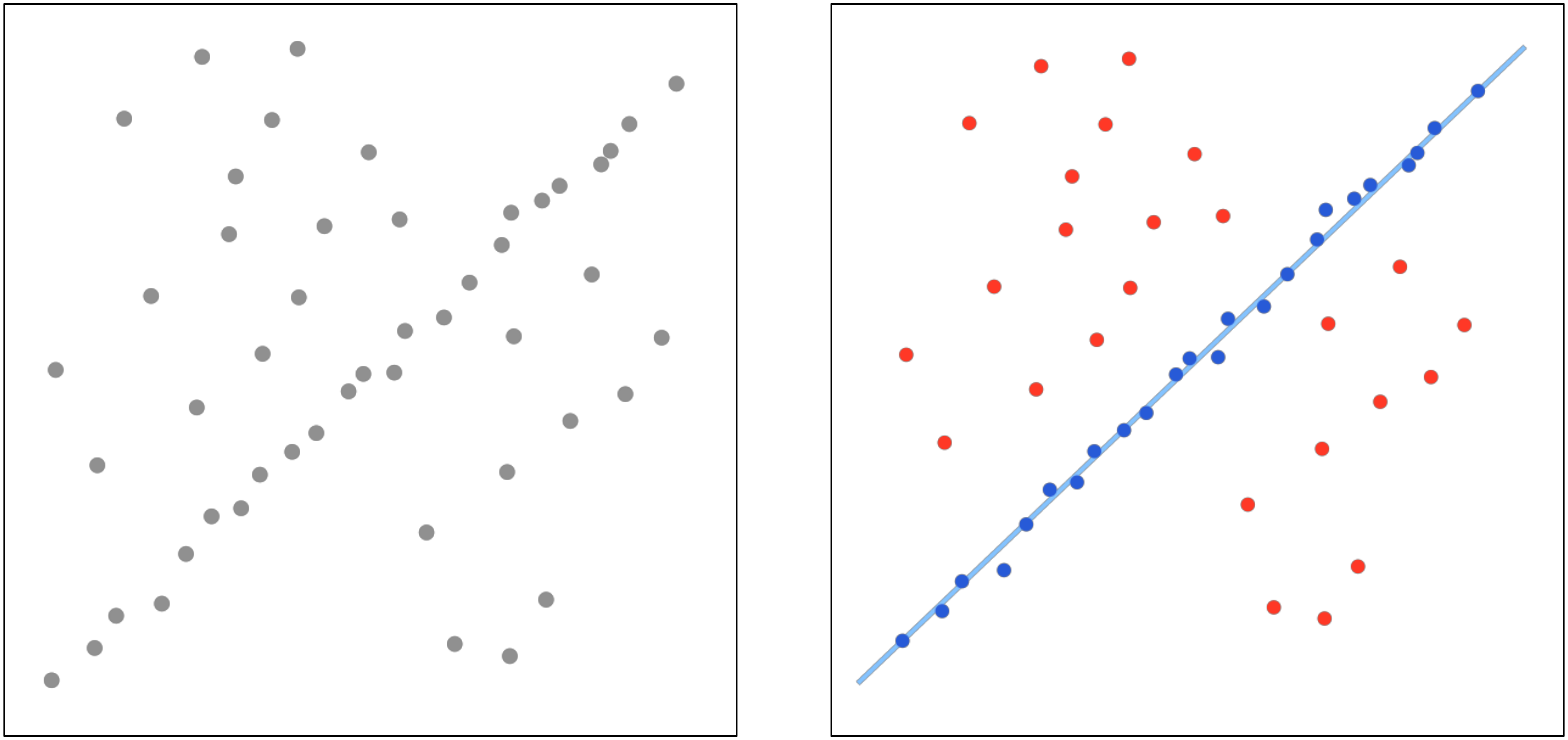
Outlier Detection and Rejection

- Special case of IRWLS: set weight = 0 if outlier, 1 otherwise
- Detecting outliers: $(y_i - f(x_i))^2 >$ threshold
  - One choice: multiple of mean squared difference
  - Better choice: multiple of *median* squared difference
  - Can iterate…
  - As before, not guaranteed to do anything reasonable, tends to work OK if only a few outliers

RANSAC

- RANdom SAmple Consensus: desgined for bad data (in best case, up to 50% outliers)
- Take many random subsets of data
  - Compute least squares fit for each sample
  - See how many points agree: $(y_i - f(x_i))^2 < \text{threshold}$
  - Threshold user-specified or estimated from more trials
- At end, use fit that agreed with most points
  - Can do one final least squares with all inliers

RANSAC



Least Squares in Practice

Least Squares in Practice

- More data is better $\sigma^2 = \dfrac{\chi^2}{n-m}\mathbf{C}$
  – uncertainty in estimated parameters goes down slowly: like 1/sqrt(# samples)
- Good correlation **doesn't mean a model is good**
  – use visualizations and reasoning, too.

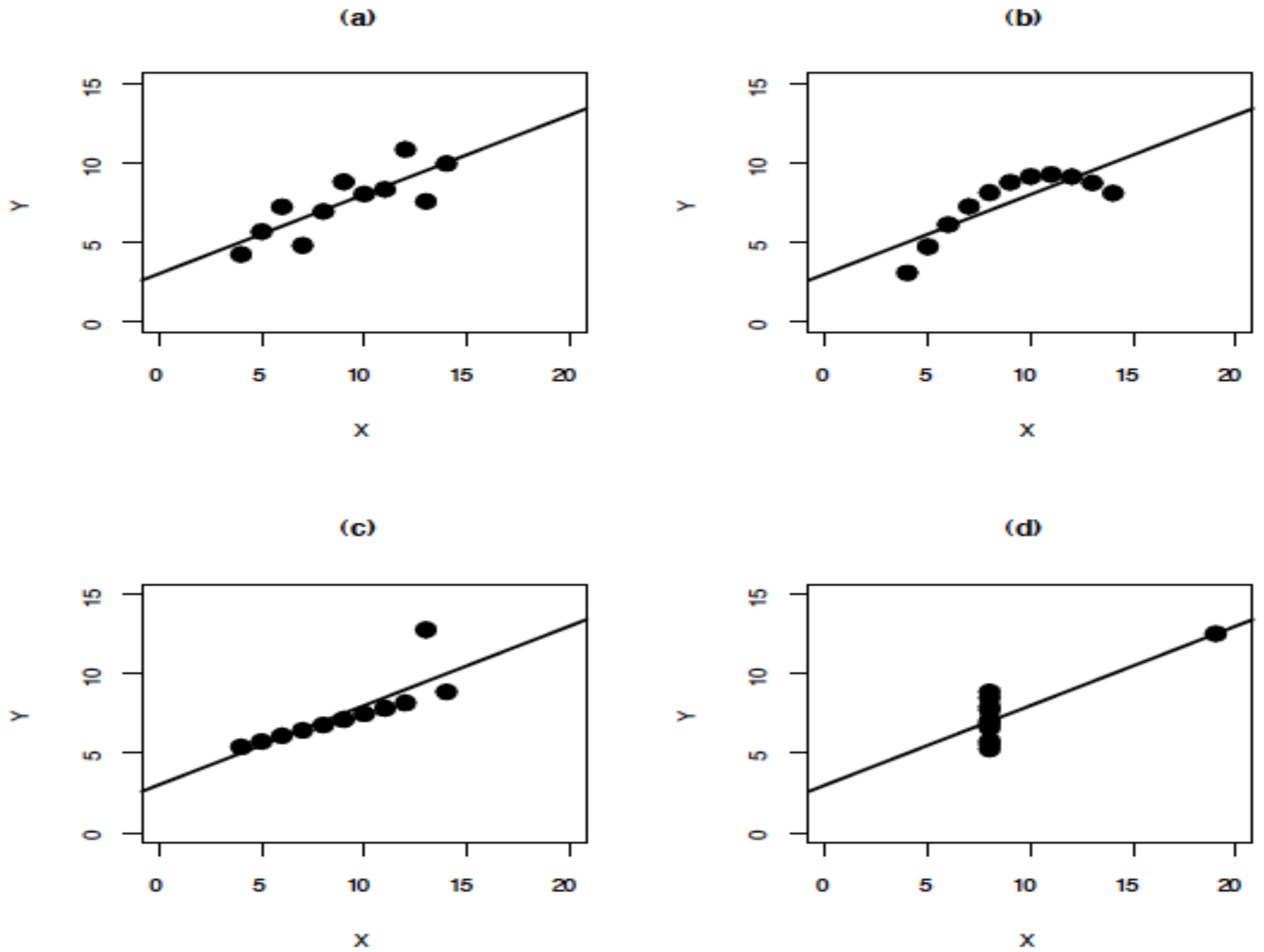
Anscombe's Quartet

Dataset 1		Dataset 2		Dataset 3		Dataset 4	
x	y	x	y	x	y	x	y
10	8.04	10	9.14	10	7.46	8	6.58
8	6.95	8	8.14	8	6.77	8	5.76
13	7.58	13	8.74	13	12.74	8	7.71
9	8.81	9	8.77	9	7.11	8	8.84
11	8.33	11	9.26	11	7.81	8	8.47
14	9.96	14	8.10	14	8.84	8	7.04
6	7.24	6	6.13	6	6.08	8	5.25
4	4.26	4	3.10	4	5.39	19	12.50
12	10.84	12	9.13	12	8.15	8	5.56
7	4.82	7	7.26	7	6.42	8	7.91
5	5.68	5	4.74	5	5.73	8	6.89

$y = 3.0 + 0.5x$

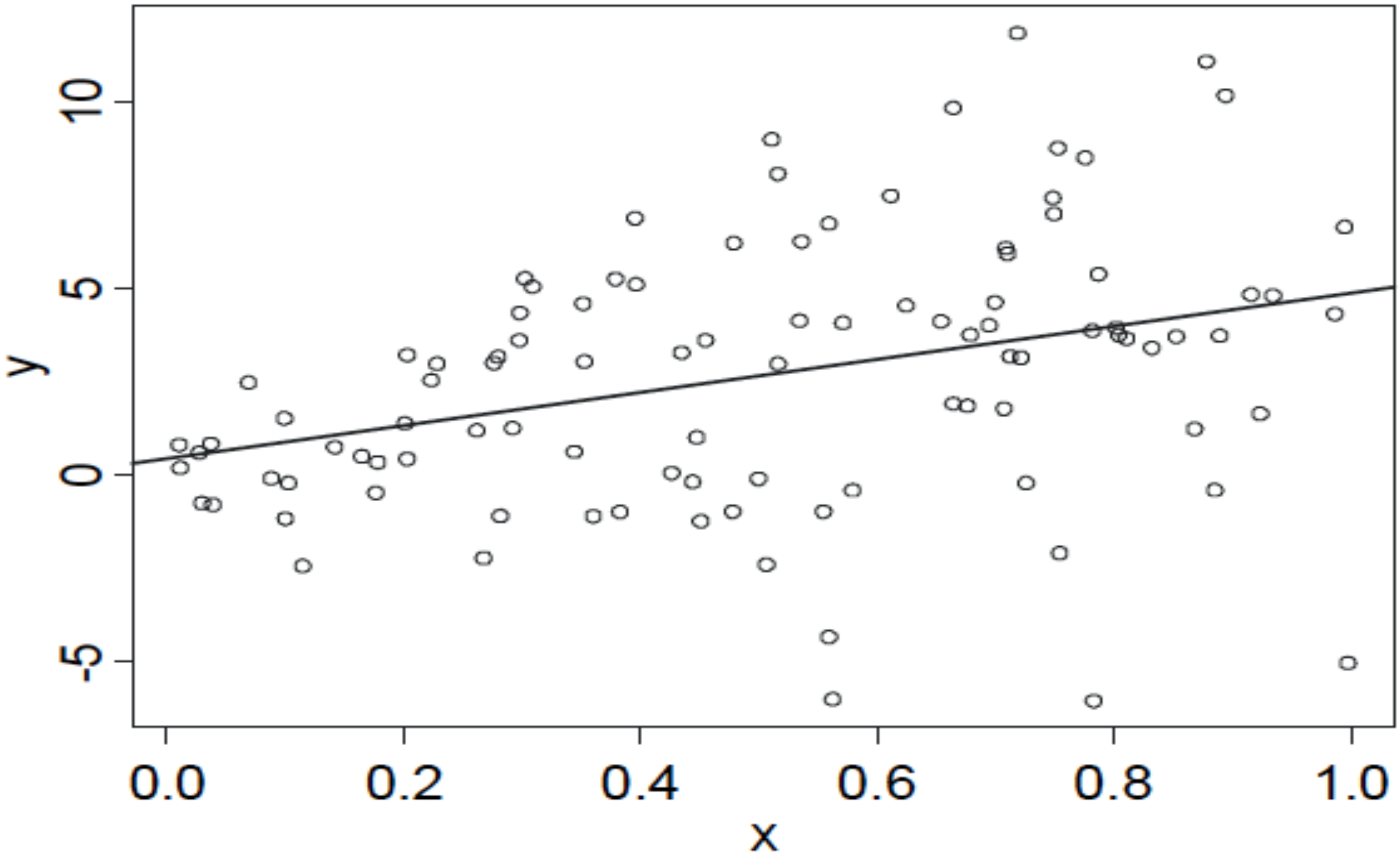
$r = 0.82$

Anscombe's Quartet



Least Squares in Practice

- More data is better
- Good correlation **doesn't mean a model is good**
- Many circumstances call for (slightly) more sophisticated models than least squares
  - Generalized linear models, regularized models (e.g., LASSO), PCA, …



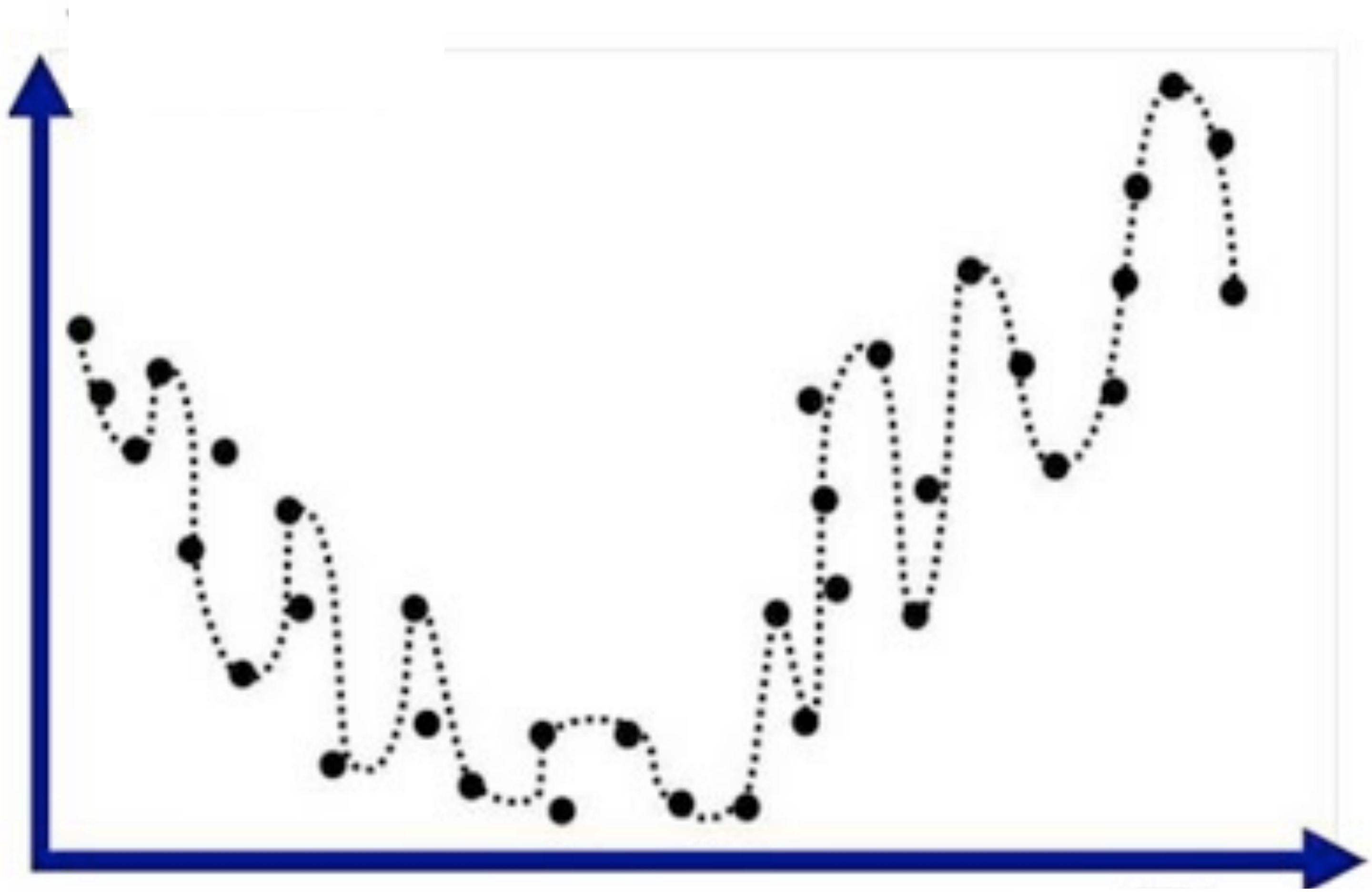
Residuals depend on x (heteroscedastic):
Assumptions of linear least squares not met

Least Squares in Practice

- More data is better
- Good correlation **doesn't mean a model is good**
- Many circumstances call for (slightly) more sophisticated models than linear LS
- Sometimes a model's fit can be **too good** ("overfitting")
  - more parameters may make it easier to overfit

$$\sigma^2 = \frac{\chi^2}{n-m}\mathbf{C}$$

Overfitting



Least Squares in Practice

- More data is better
- Good correlation **doesn't mean a model is good**
- Many circumstances call for (slightly) more sophisticated models than linear LS
- Sometimes a model's fit can be **too good**
- All of these minimize "vertical" squared distance
  - Square, vertical distance not always appropriate

Least Squares in Matlab, Excel

- Matlab
  - Linear L.S.: **polyfit**
    - For polynomial of arbitrary degree
    - Plot/use with **polyval**
  - Non-linear:
    - **lsqnonlin**, **lsqcurvefit**
    - **fminsearch** (generic optimization, uses simplex)
  - Curve fitting toolbox, Optimization toolbox
- Excel: Chart trendlines use least squares