6.7900: Machine Learning
Lecture 4

Lecture start: Tues/Thurs 2:35pm
Who's speaking today? Prof. Tamara Broderick
Course website: gradml.mit.edu
Questions? Ask here or on piazza.com/mit/fall2024/67900/
Materials: Slides, video, etc linked from gradml.mit.edu after the lecture (but there is no livestream)

Last Times

I. Empirical risk minimization (ERM)
II. Maximum likelihood estimate (MLE)
III. No features

Today's Plan

I. MLE & ERM for supervised learning
II. Linear regression: Why and how
III. Some challenges

Why linear regression?

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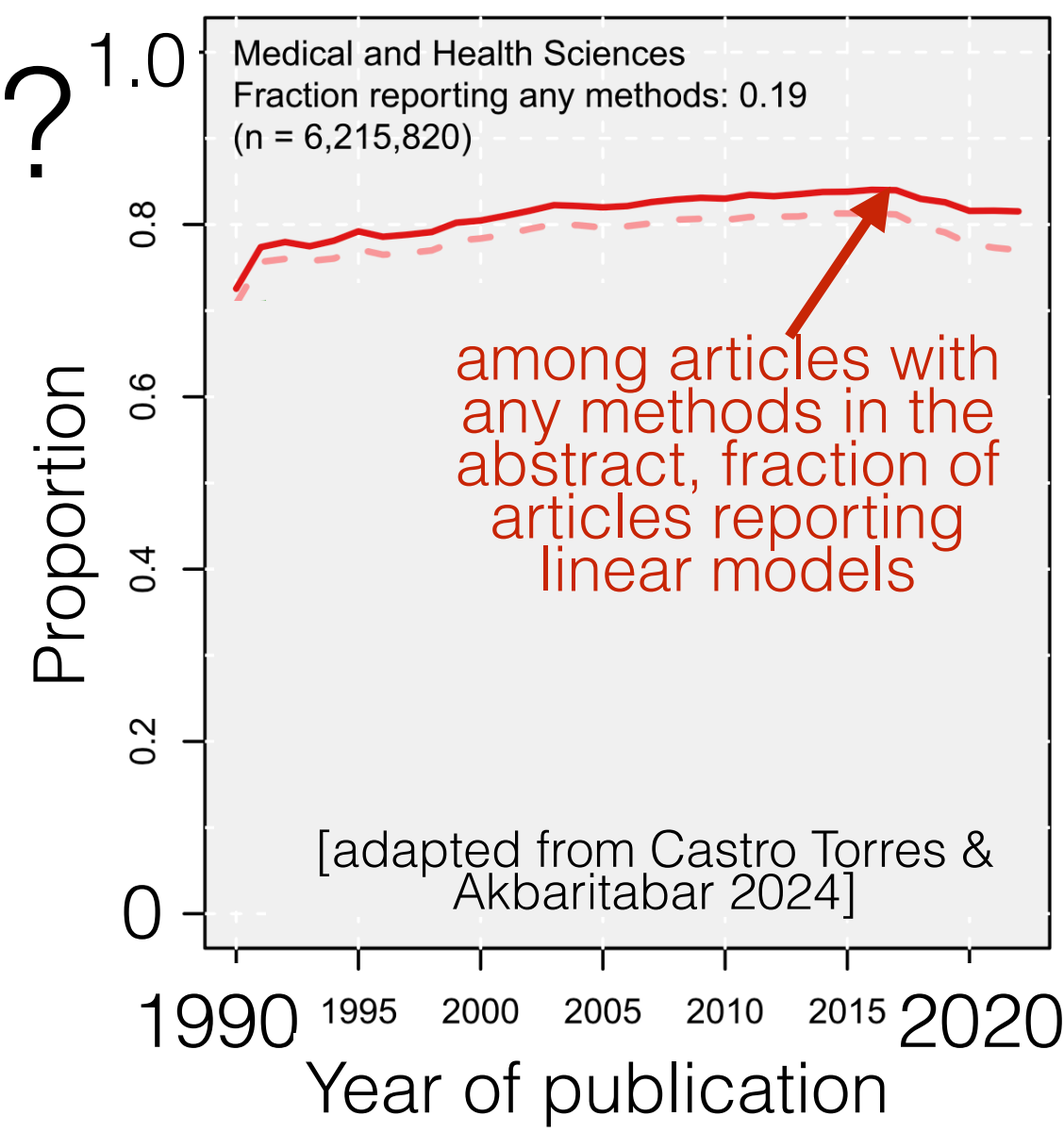

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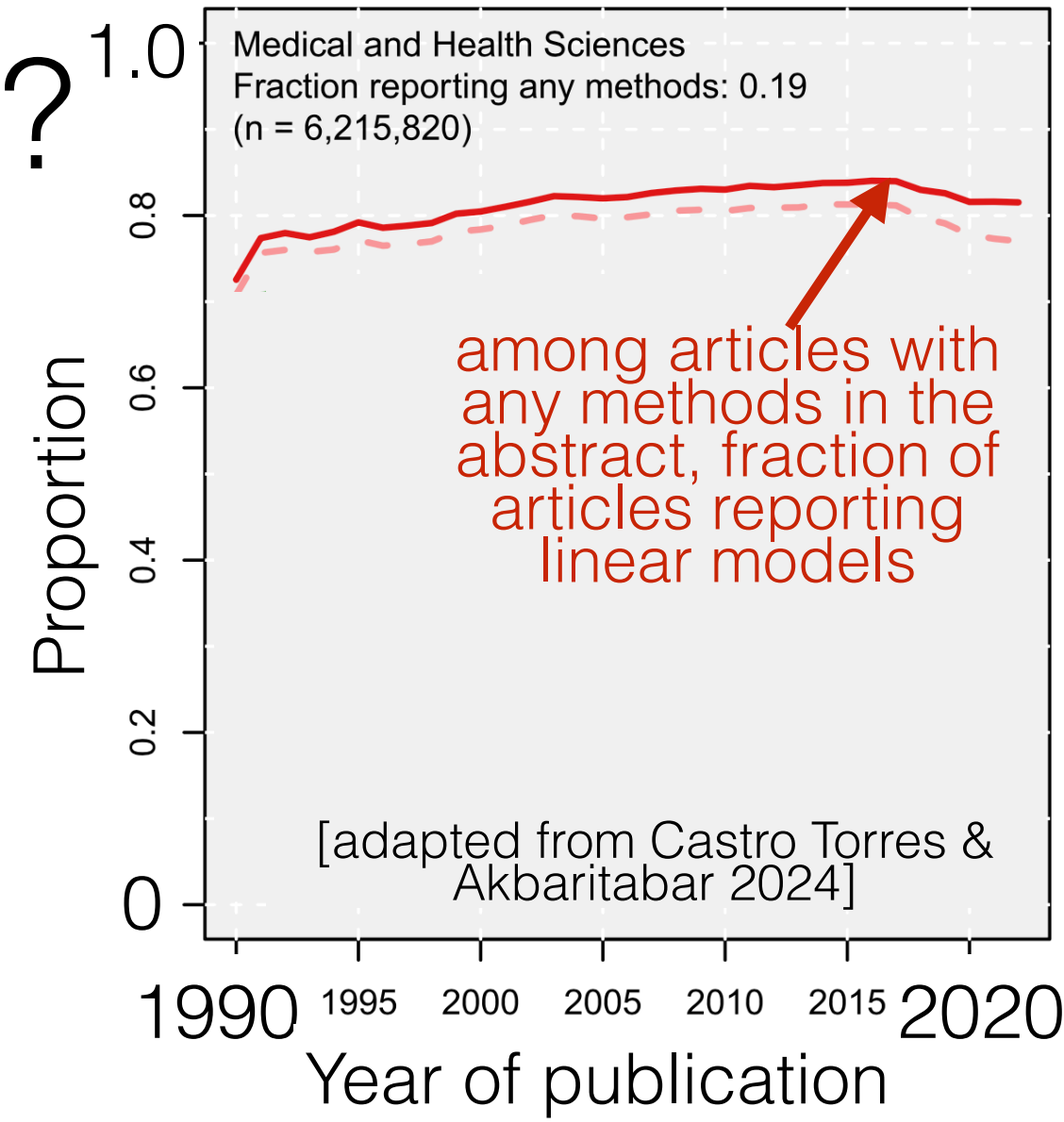
- Speed, interpretability



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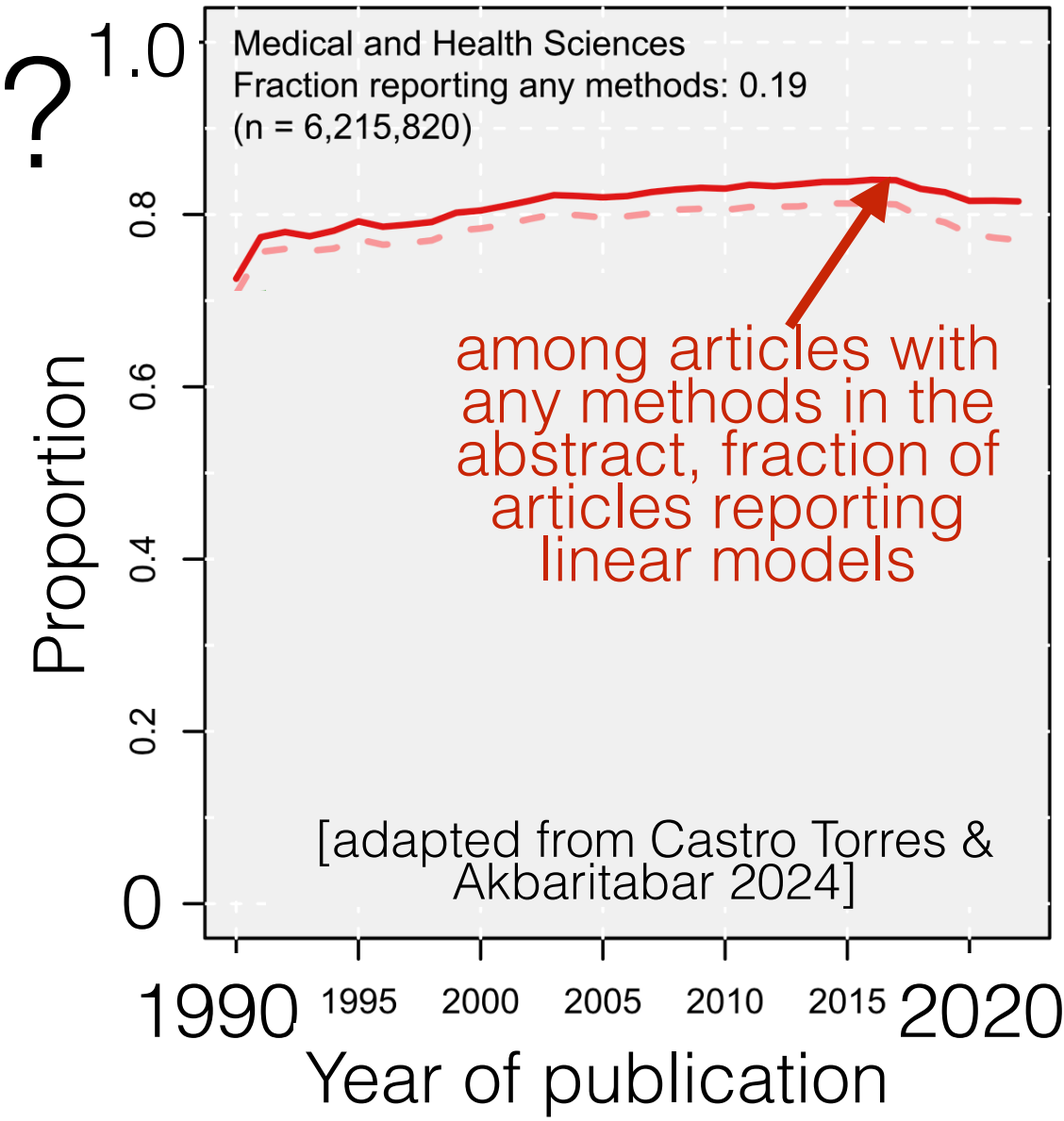
[e.g. Bartlett+ 2020, Benign overfitting in linear regression]



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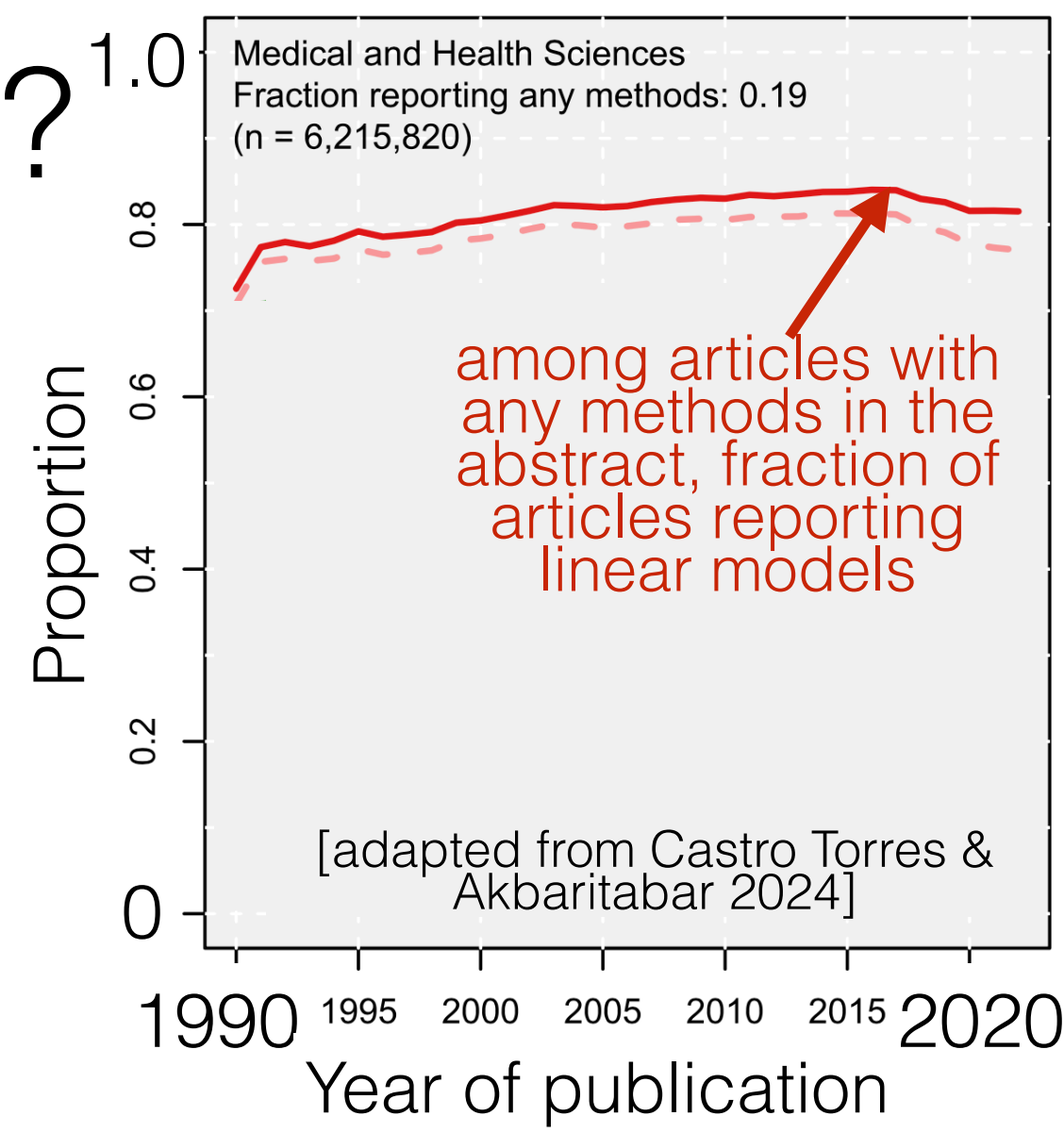

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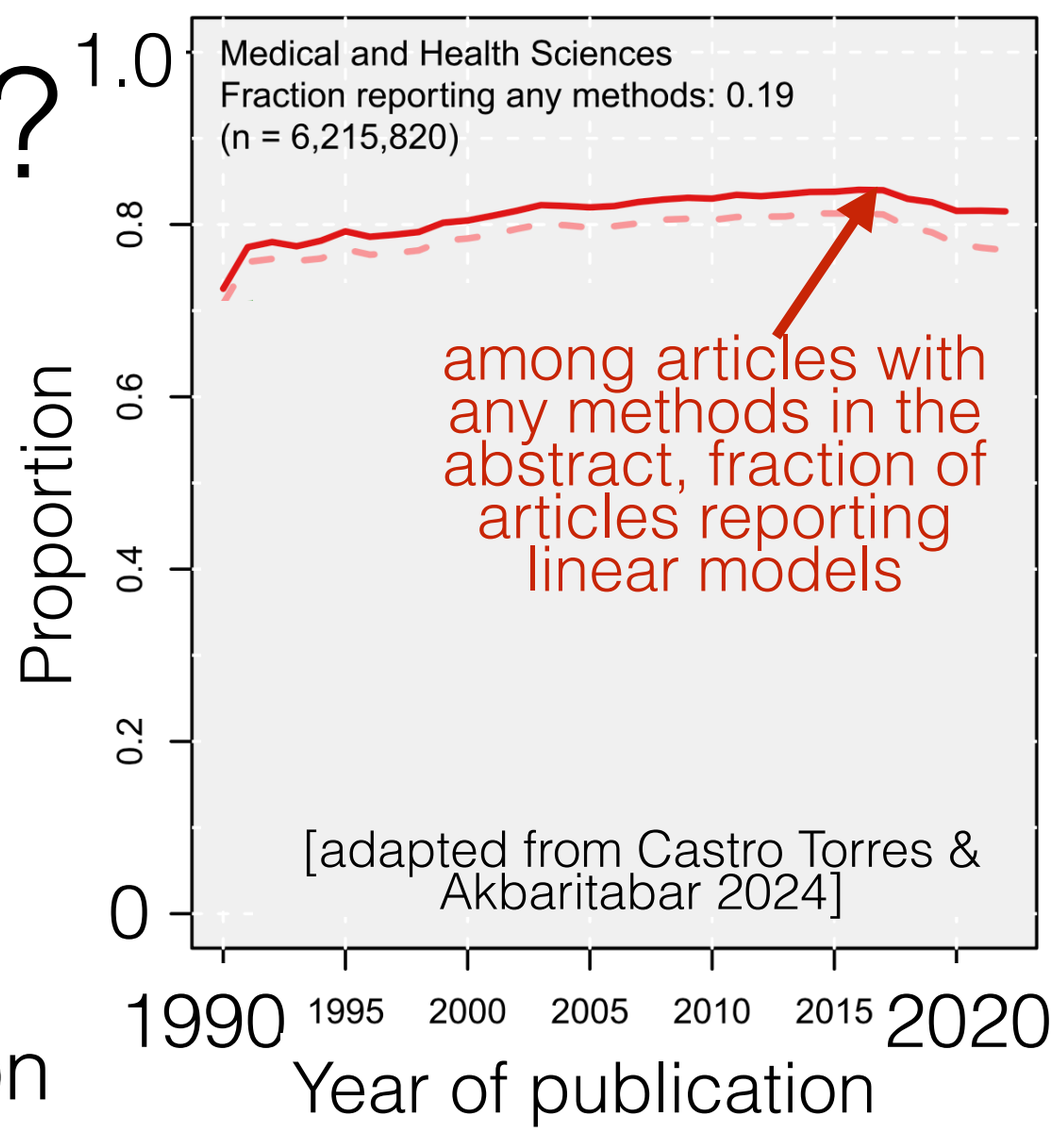

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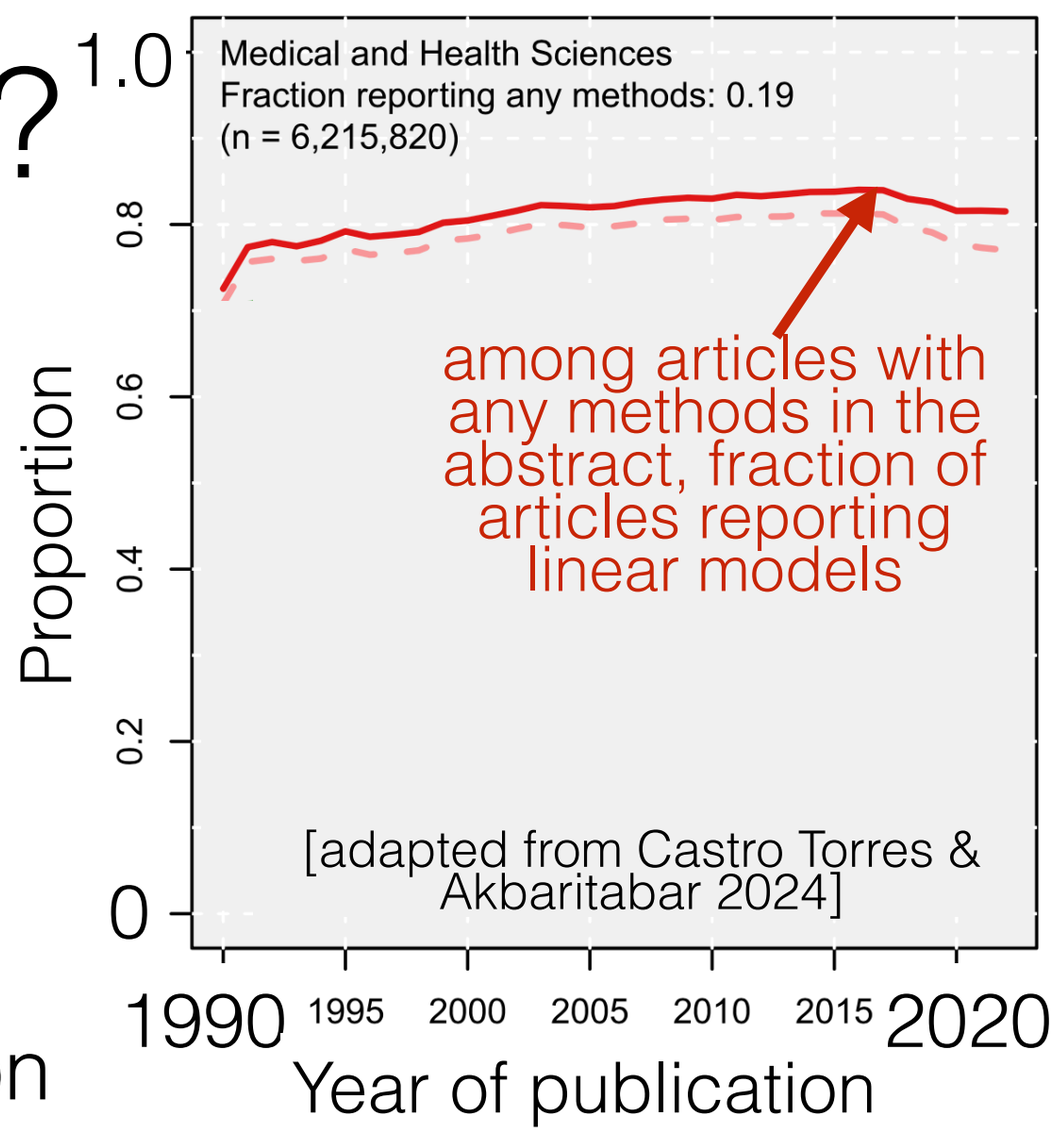

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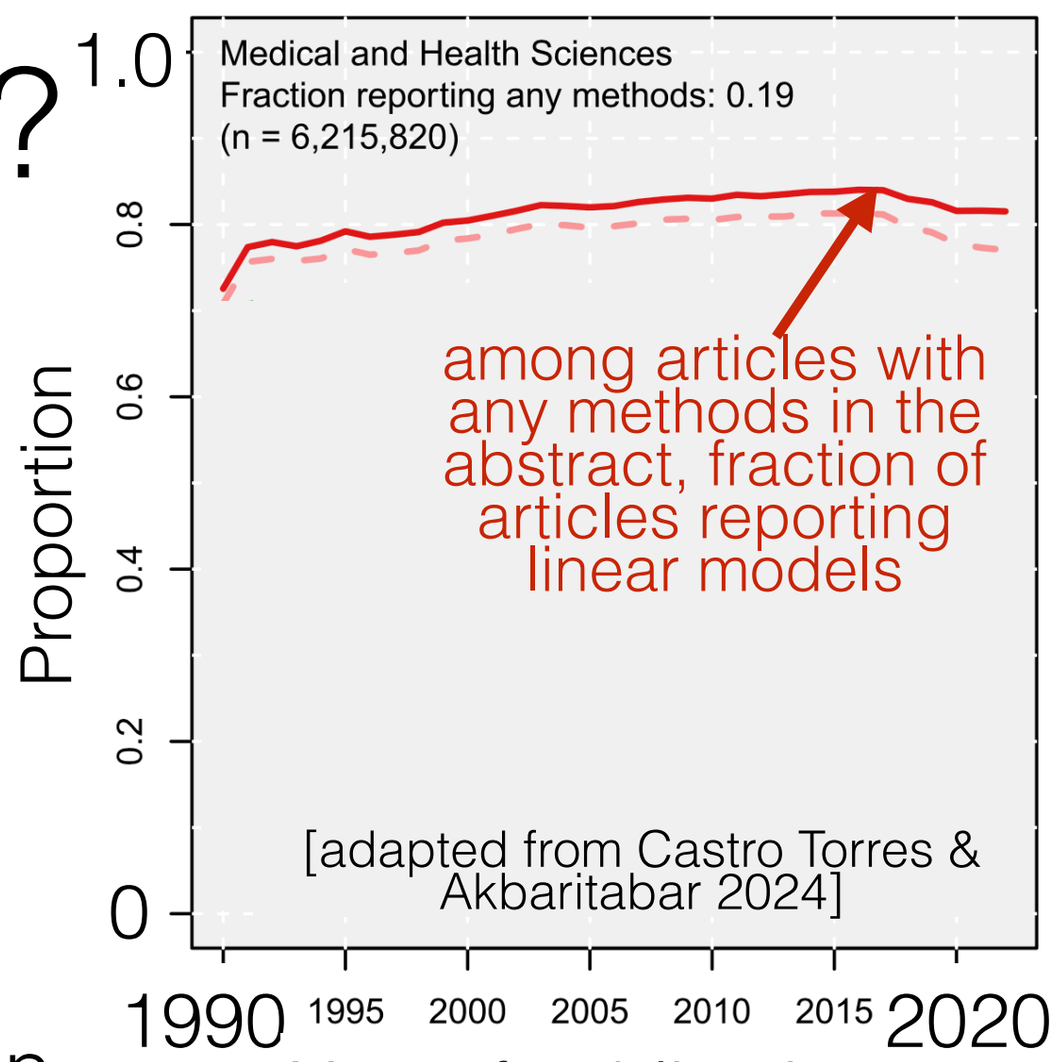

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  - Chen et al 2016, A Thorough Examination of the CNN/Daily Mail Reading Comprehension Task

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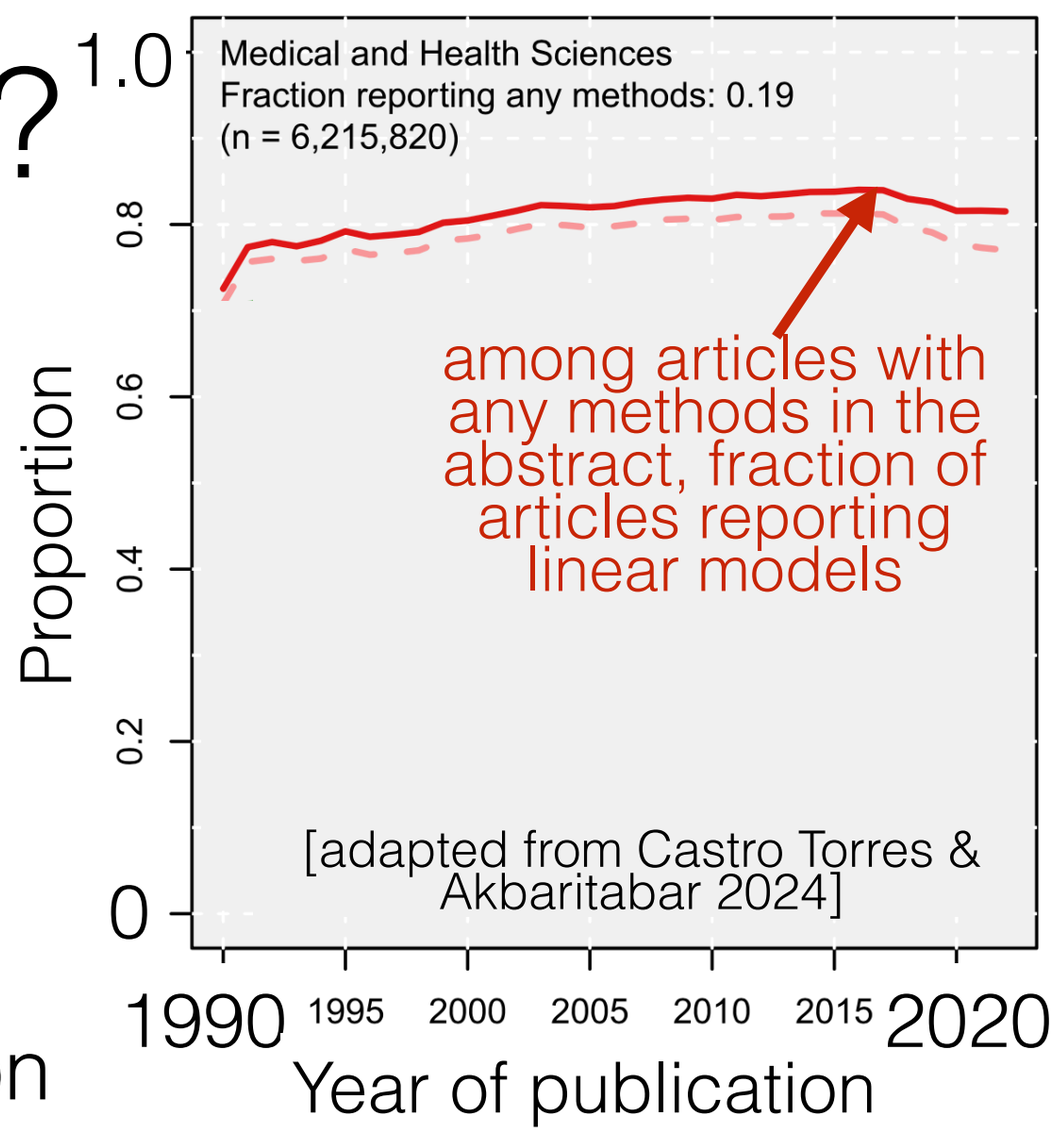

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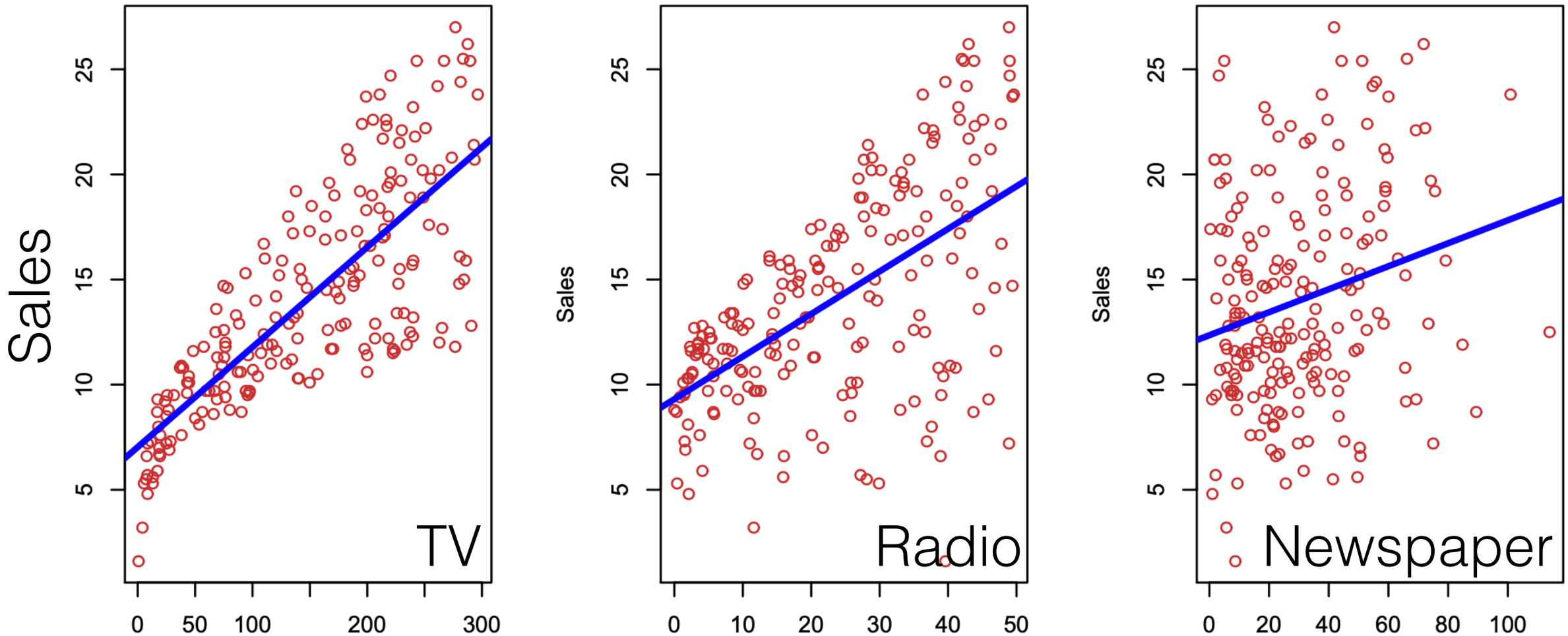
[An Intro to Statistical Learning 2023, Fig 2.1]



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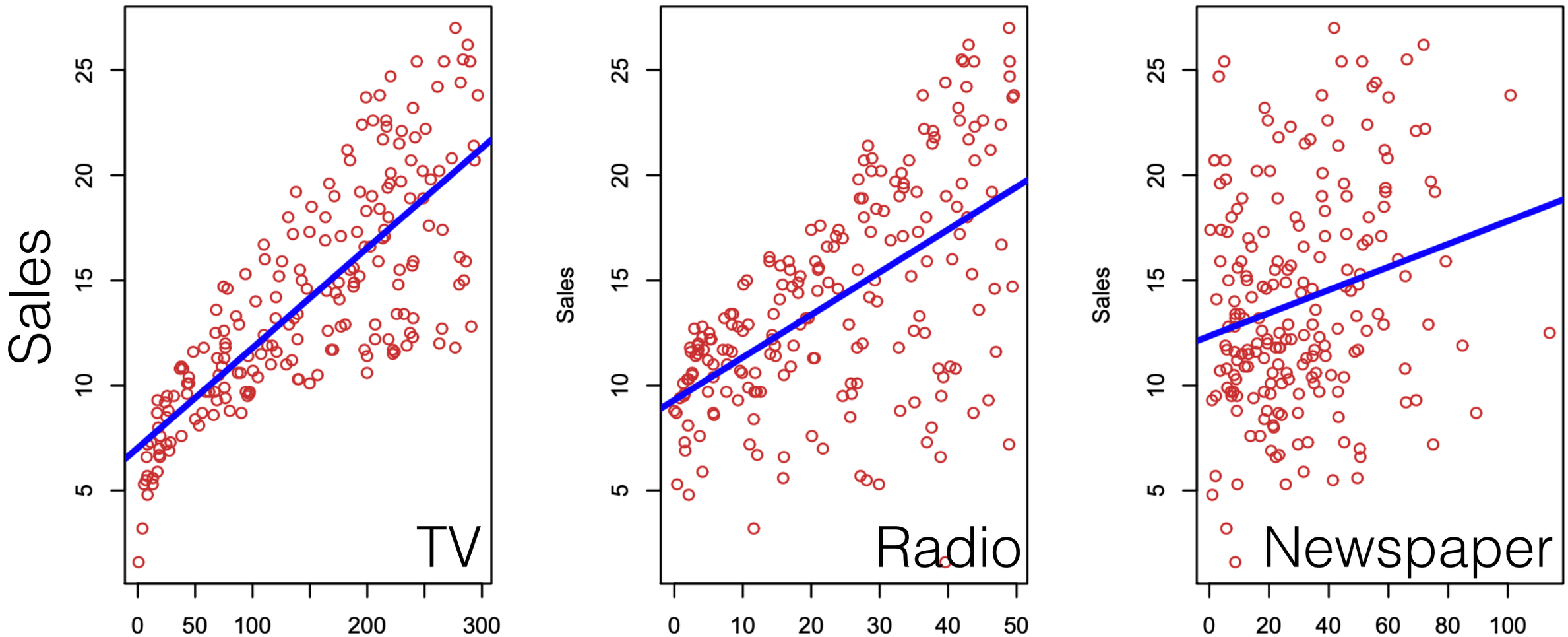

- Data point: label is sales, in thousands of units: $y^{(n)} \in \mathbb{R}_+$
  - Features: $x^{(n)} = [x_1^{(n)}, x_2^{(n)}, x_3^{(n)}]^\top \in \mathbb{R}_+^3$

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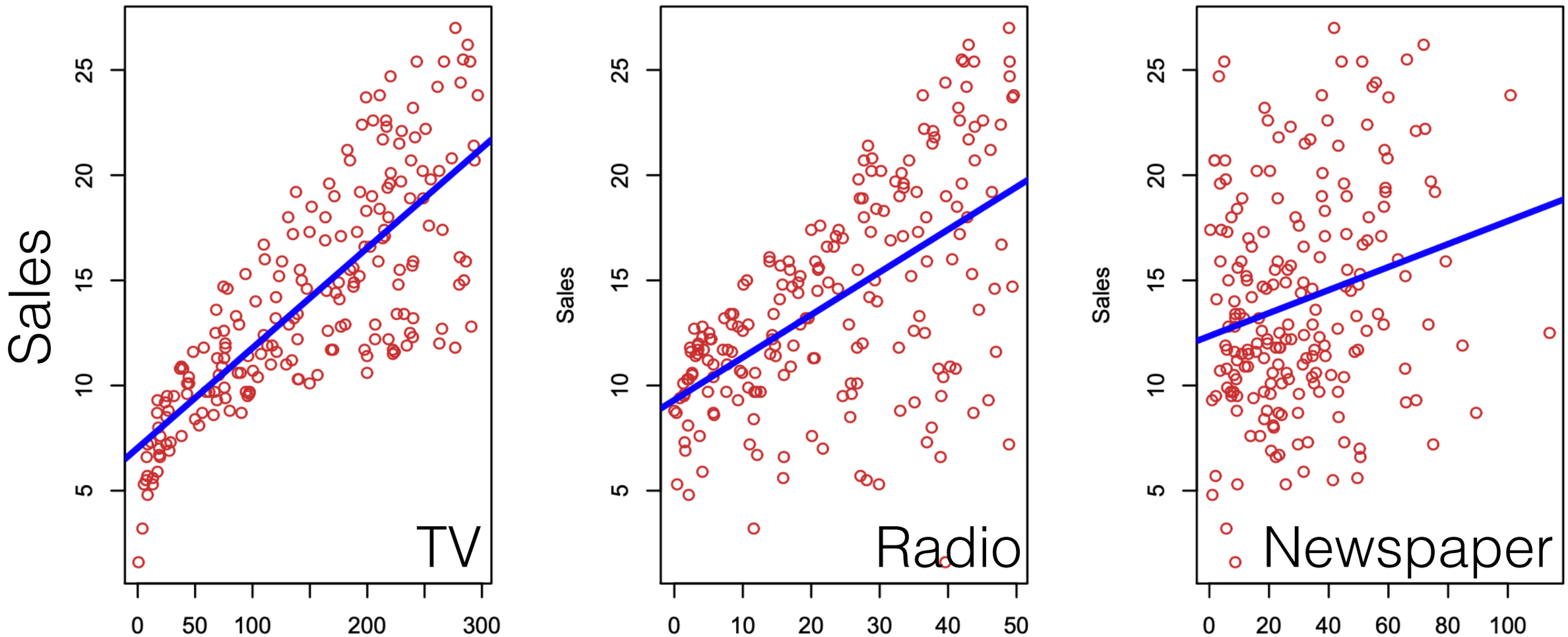

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  - Features: $x^{(n)} = [x_1^{(n)}, x_2^{(n)}, x_3^{(n)}]^\top \in \mathbb{R}_+^3$
- Want to predict sales under different ad budgets, allocate ad budget. Separate regressions not same as whole.

Choosing a likelihood

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  (1x1 = $y^{(n)}$, 1xD = $\theta^\top$, Dx1 = $x^{(n)}$, 1x1 = $\epsilon^{(n)}$, 1x1 = $\mathcal{N}(0, \sigma^2)$)
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fit params $= \arg\max p(\{y^{(n)}\}_1^N | \{x^{(n)}\}_1^N,$ parameters?)

parameters

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$$\hat{\theta}, \hat{\sigma}^2 = \arg\max_{\theta, \sigma^2} p(\{y^{(n)}\}_1^N | \{x^{(n)}\}_1^N, \theta, \sigma^2)$$

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    - Can handle an intercept term by taking: $\forall n, x_1^{(n)} = 1$
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$$p(y|x, \theta, \sigma^2) = \mathcal{N}(y|\theta^\top x, \sigma^2)$$

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homoskedastic noise

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$\underbrace{\qquad\qquad\qquad\qquad\qquad\qquad}_{\text{Residual sum of squares (RSS)}}$

- The **residual** is a more general concept: $y^{(n)} - h(x^{(n)})$

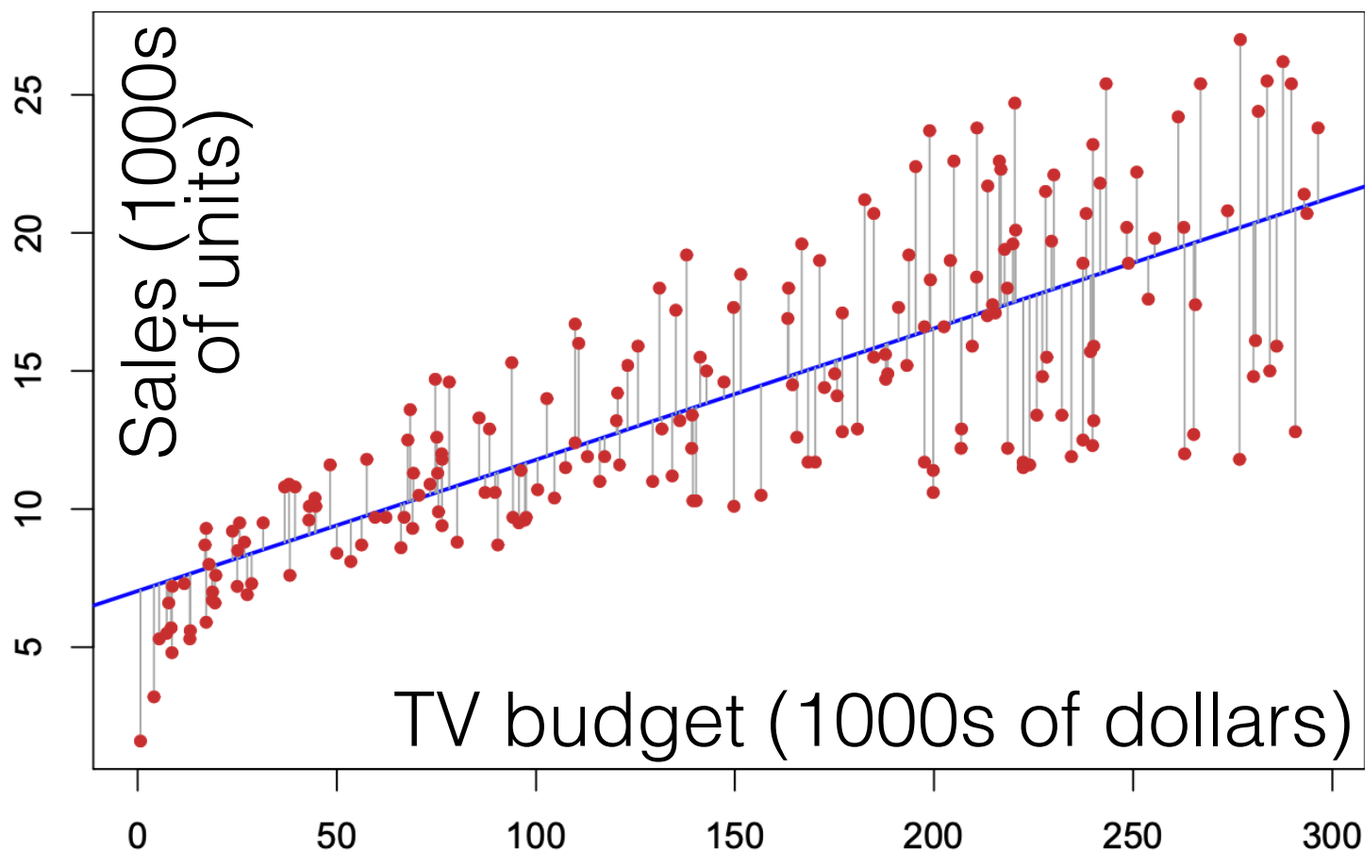
Some visualizations

6a

Some visualizations

- Linear predictor and residuals for one feature (with an intercept)

Some visualizations



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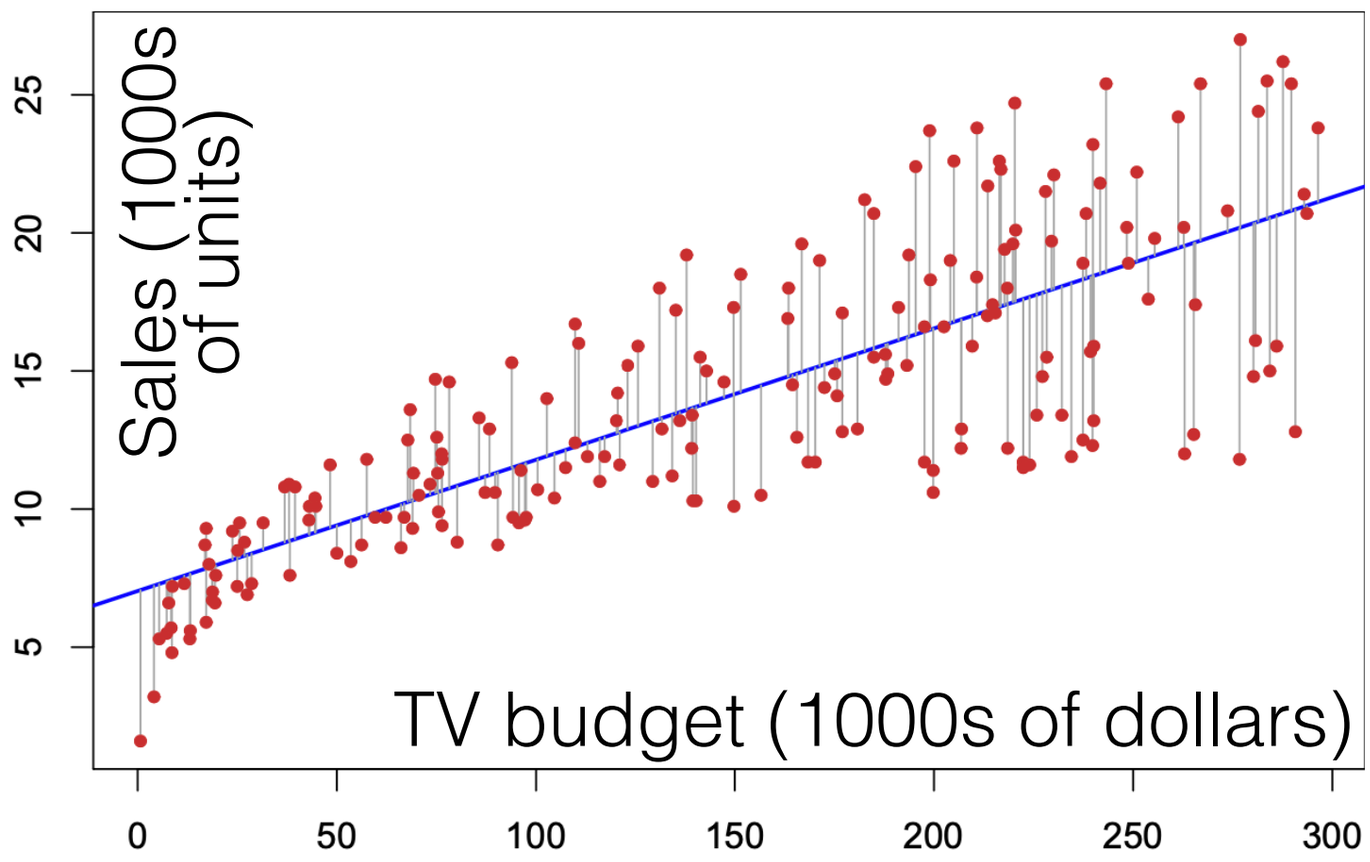
[An Intro to Statistical Learning 2023, Fig 3.1]

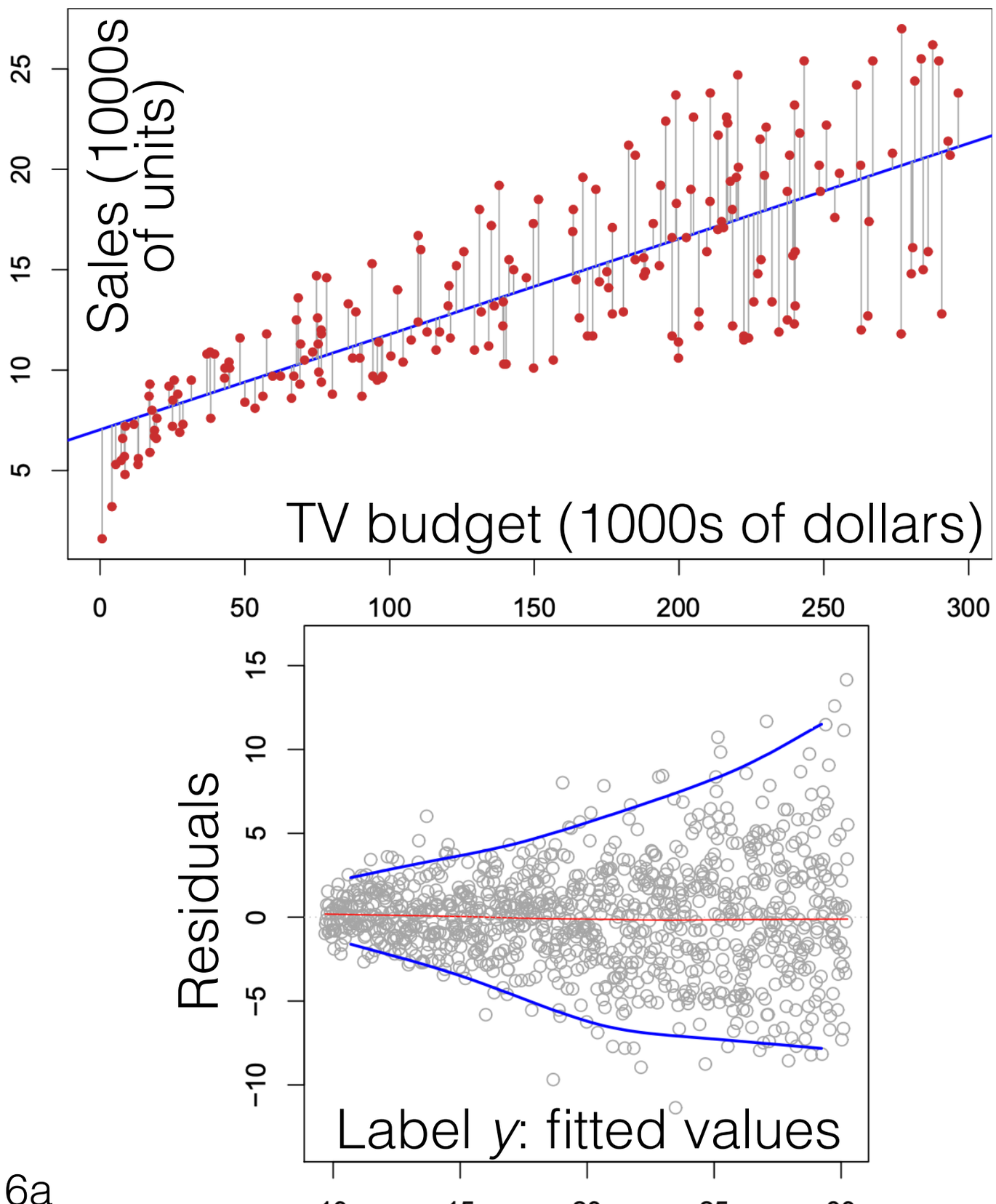
Some visualizations



- Linear predictor and residuals for one feature (with an intercept)
- Can use residual plots of the fitted predictor to check model assumptions

[An Intro to Statistical Learning 2023, Fig 3.1]

Some visualizations



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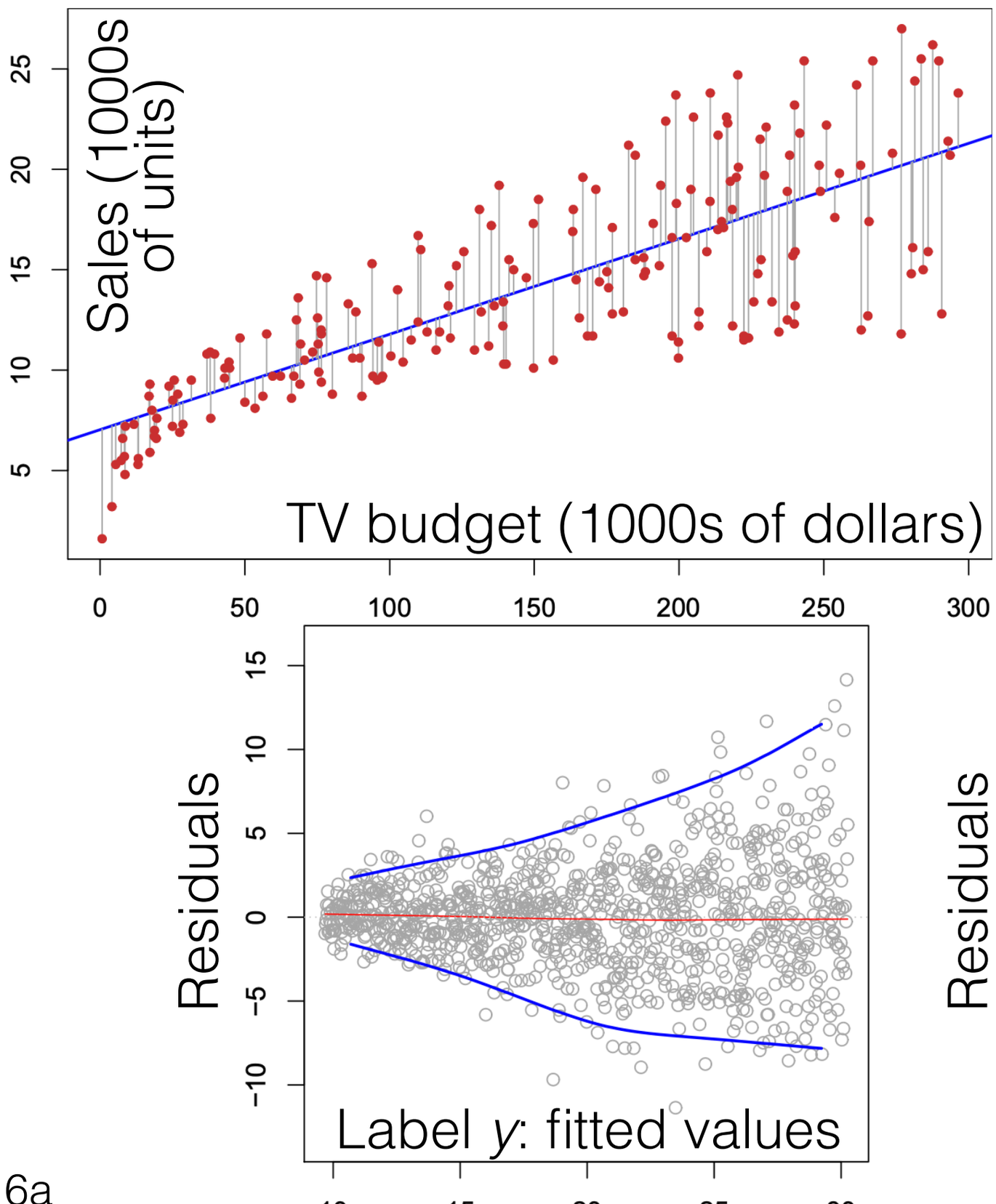
[An Intro to Statistical Learning 2023, Figs 3.1 and 3.11]

Some visualizations



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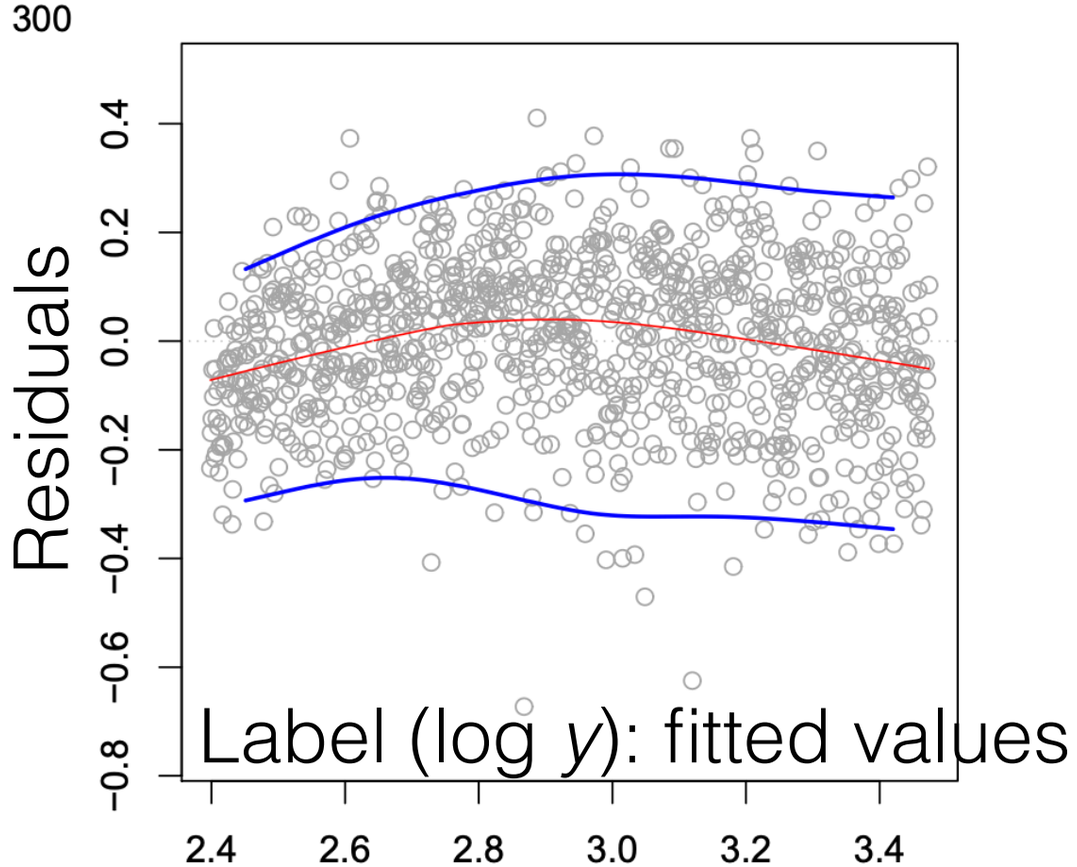

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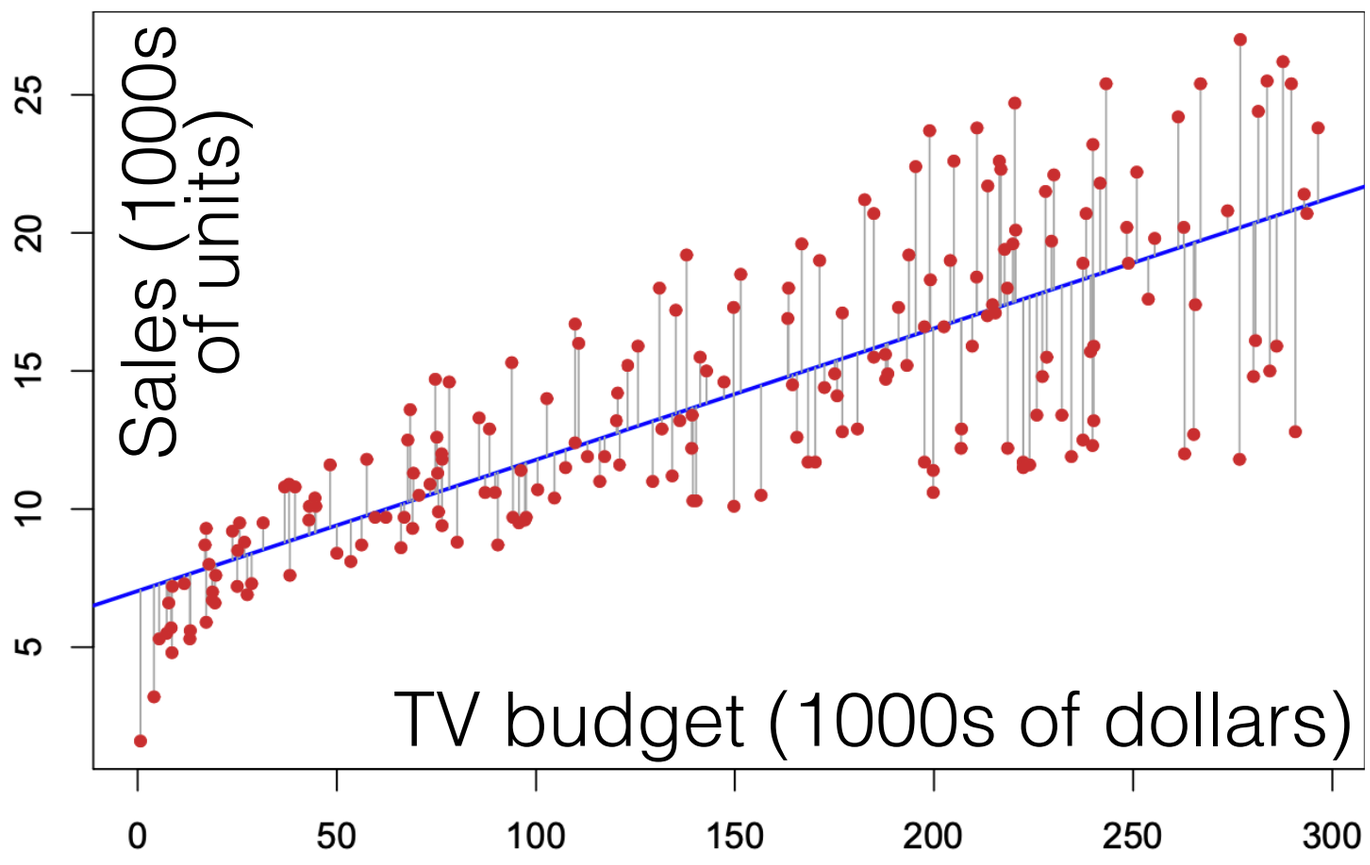

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[An Intro to Statistical Learning 2023, Fig 3.1]

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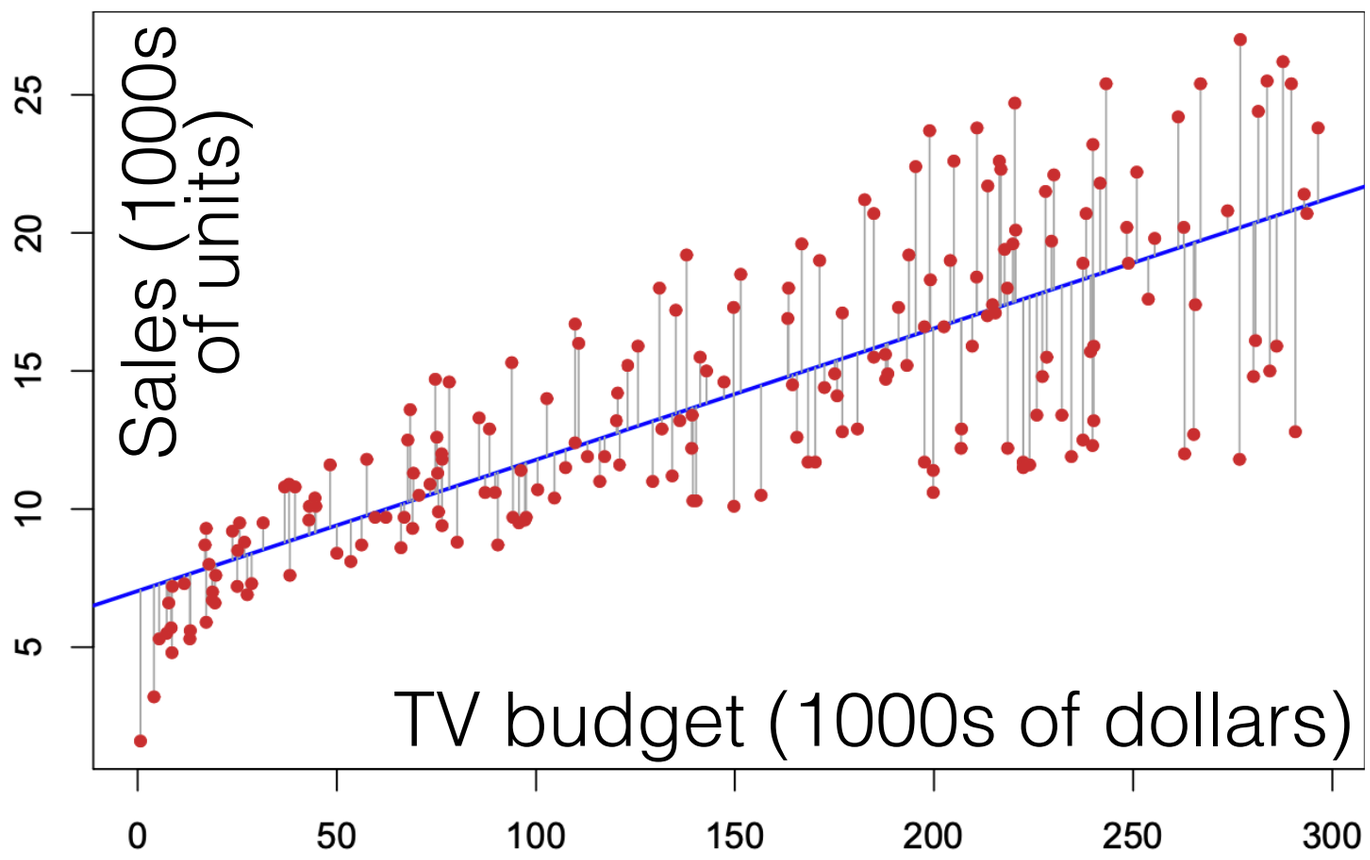

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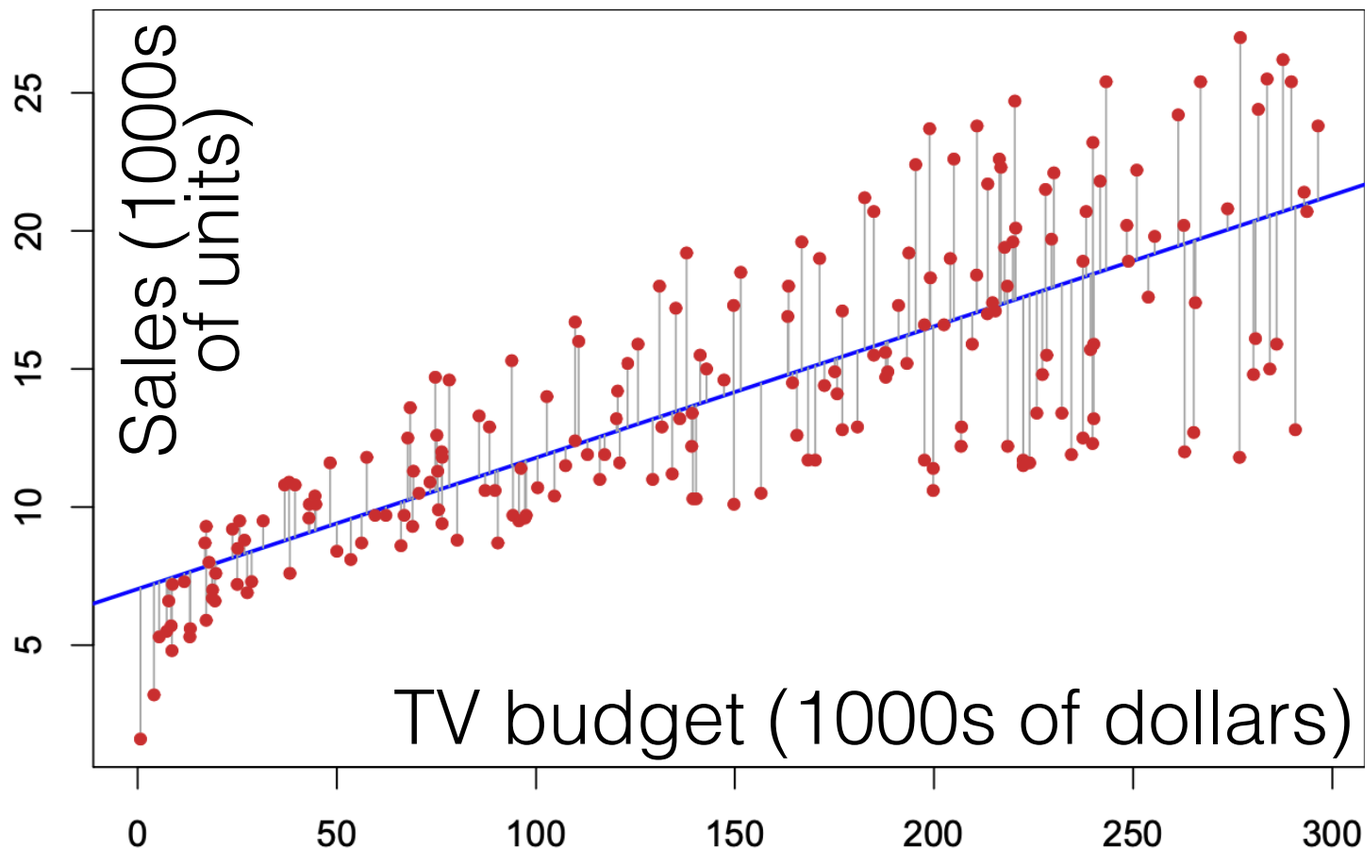
[An Intro to Statistical Learning 2023, Fig 3.1]

- Linear predictor & residuals for two features (with an intercept term)

Some visualizations



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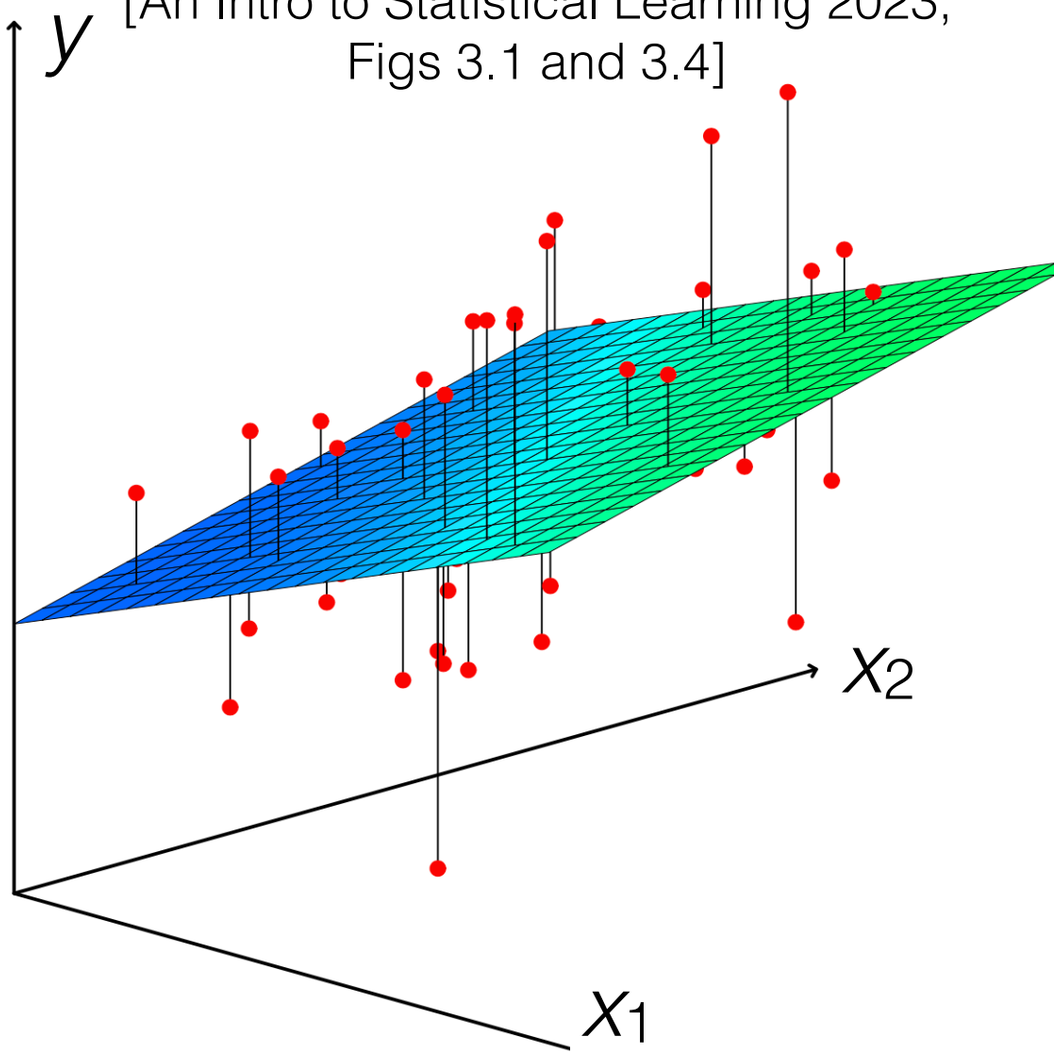
[An Intro to Statistical Learning 2023, Figs 3.1 and 3.4]



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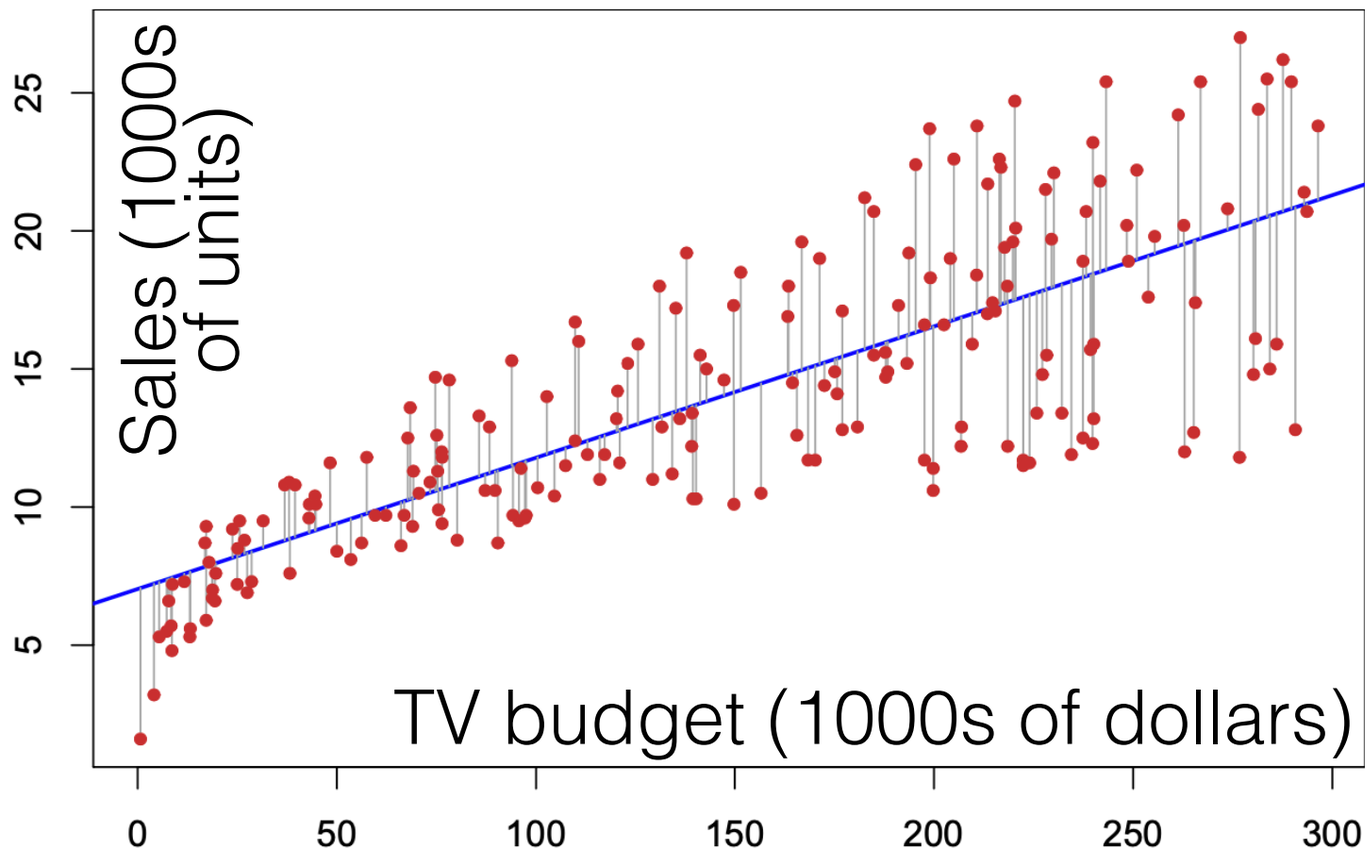

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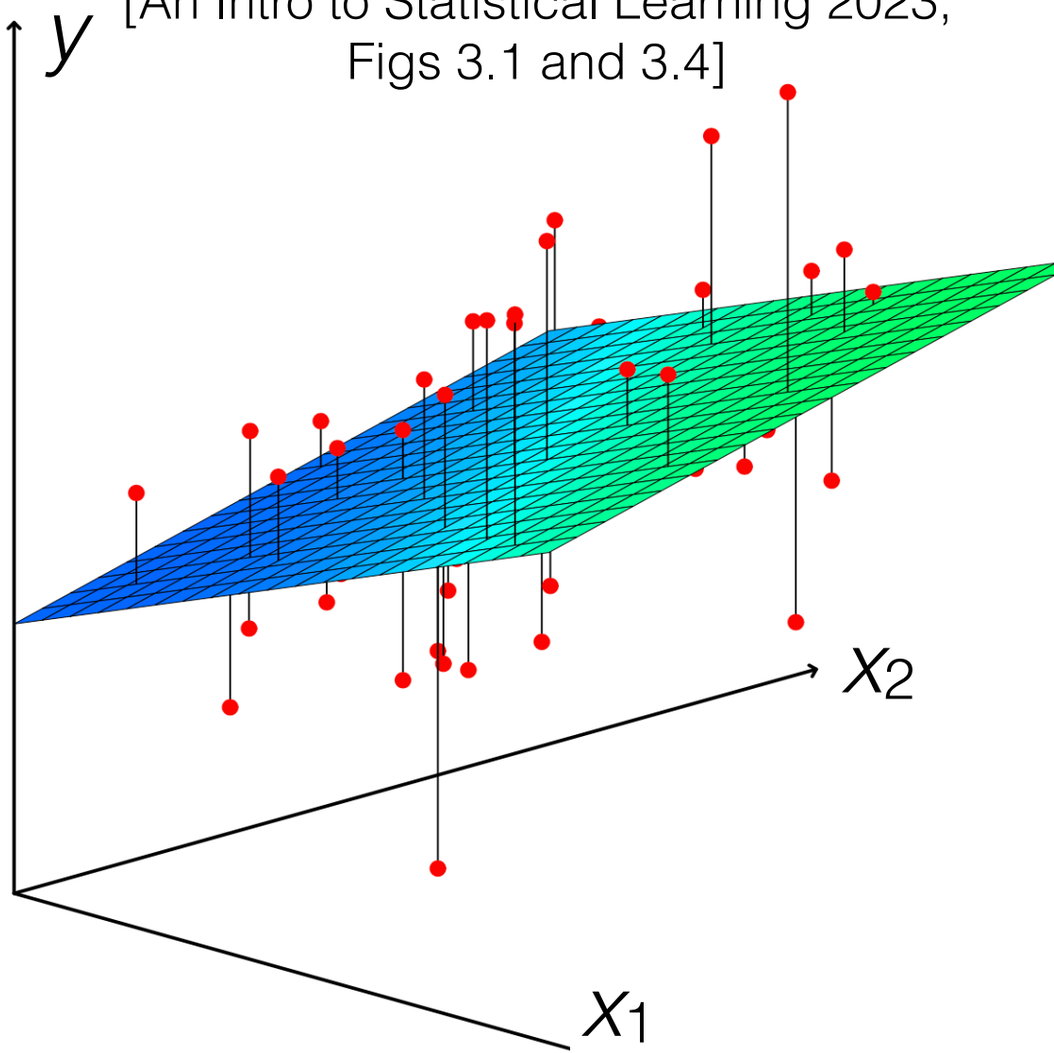
[An Intro to Statistical Learning 2023, Figs 3.1 and 3.4]



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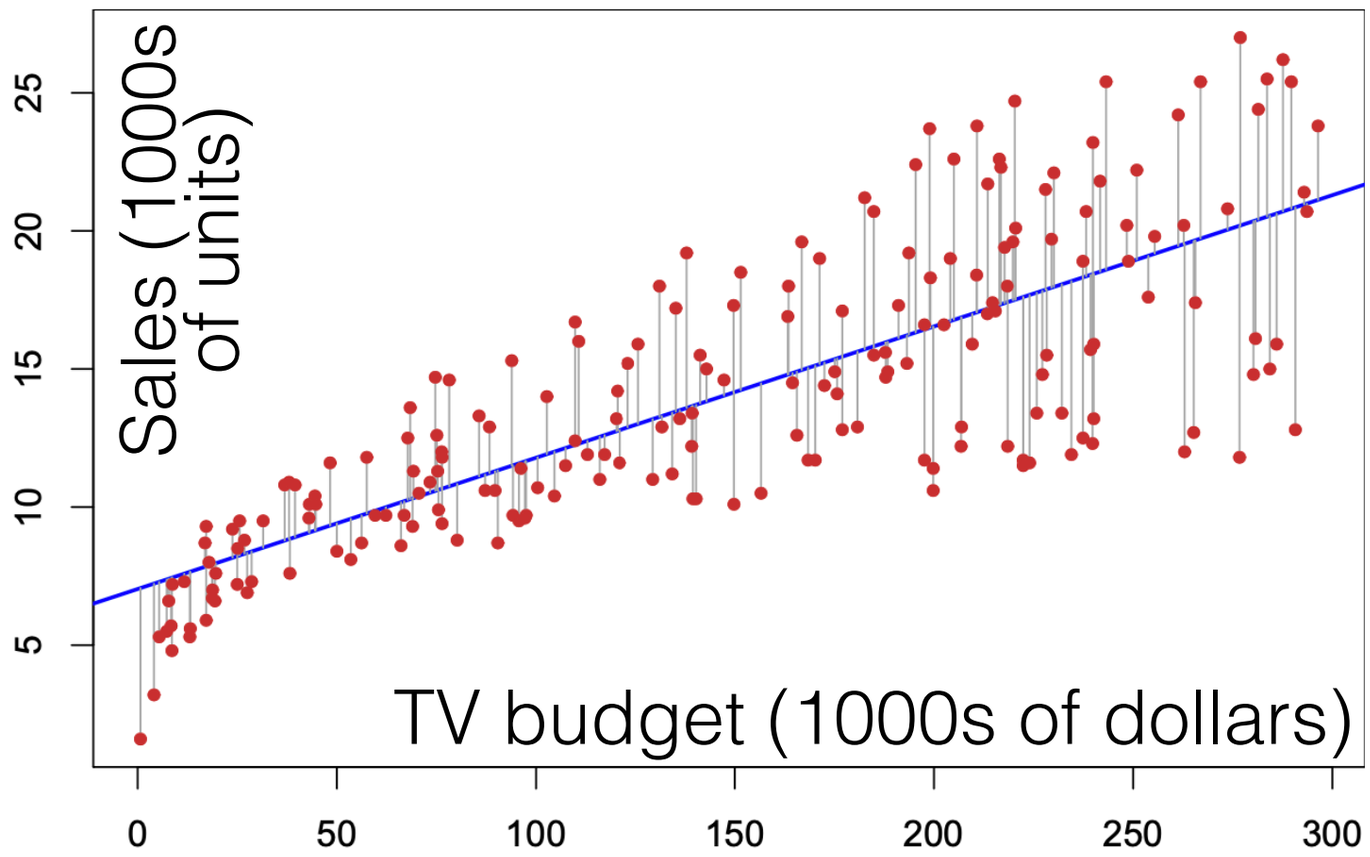

- Linear predictor & residuals for two features (with an intercept term)
- In general, $\theta^\top x$ is a hyperplane (one dim less than (*x,y*) space)
- Check: regressing label on the features is not equivalent to regressing one feature on label and remaining features

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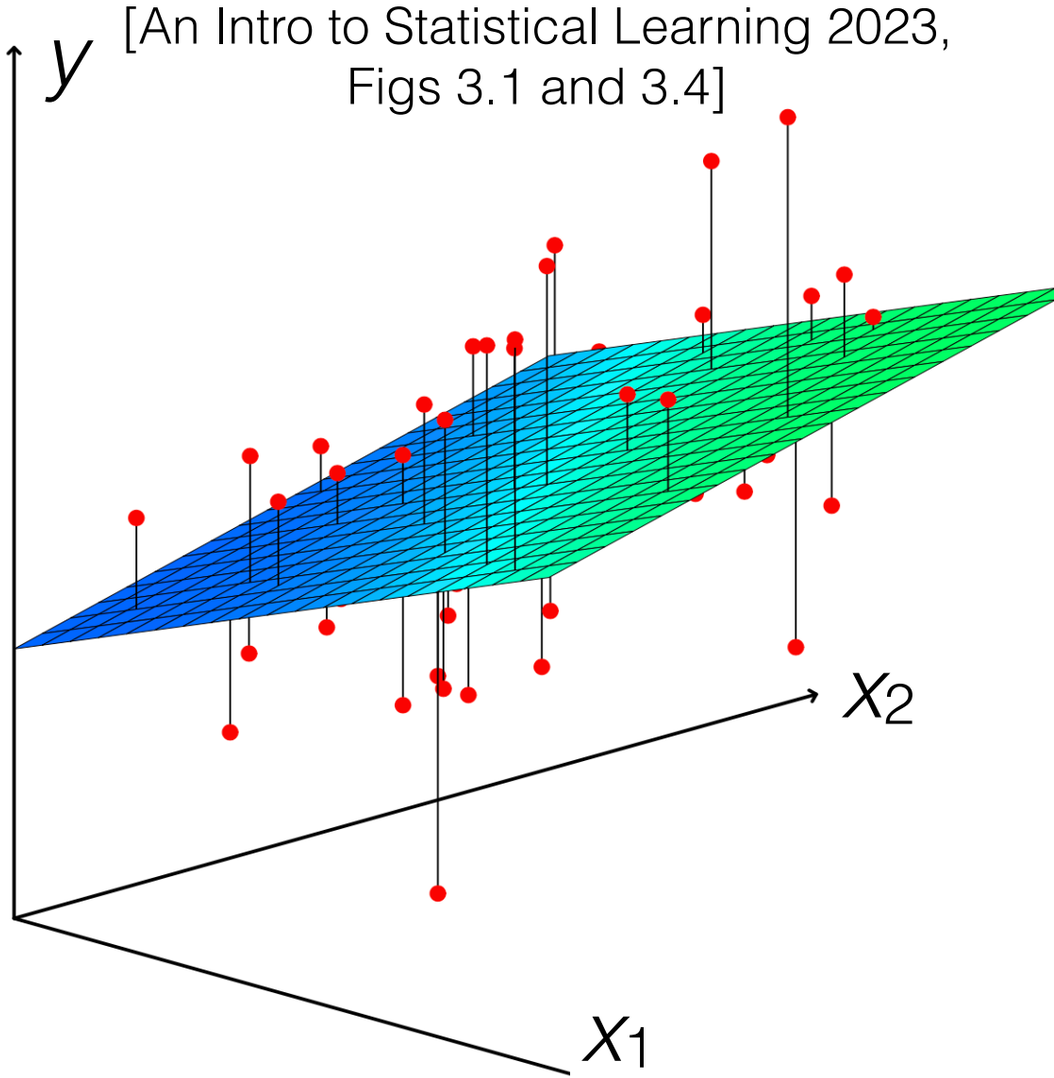
[An Intro to Statistical Learning 2023, Figs 3.1 and 3.4]



Empirical risk minimization

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    same objective from maximum likelihood! (up to a constant factor)

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    same objective from maximum likelihood! (up to a constant factor)

    - relation is specific to this model

Empirical risk minimization

- Empirical risk for square loss:

$$\frac{1}{N}\sum_{n=1}^{N} L(y^{(n)}, h(x^{(n)})) = \frac{1}{N}\sum_{n=1}^{N} (y^{(n)} - h(x^{(n)}))^2$$

  - Still not useful if we allow all decision rules (functions) *h*

- What if we instead allow only linear predictors: $h(x) = \theta^\top x$
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- Notation:

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- Notation:

$$X = \begin{pmatrix} (x^{(1)})^\top \\ (x^{(2)})^\top \\ \vdots \\ (x^{(N)})^\top \end{pmatrix}$$

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- Notation:

$$X = \underset{\text{NxD}}{\begin{pmatrix} (x^{(1)})^\top \\ (x^{(2)})^\top \\ \vdots \\ (x^{(N)})^\top \end{pmatrix}}$$

Dx1

Empirical risk minimization

- Empirical risk for square loss:

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- relation is specific to this model

- Notation:

$$Y = [y^{(1)}, y^{(2)}, \cdots, y^{(N)}]^\top$$

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Dx1

- Then $\mathrm{RSS}(\theta) =$

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Nx1

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Dx1

- Then $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$

Empirical risk minimization

- Empirical risk for square loss:

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Mean squared error (MSE)

same objective from maximum likelihood! (up to a constant factor)

- relation is specific to this model

- Notation:

$$X = \underset{\text{NxD}}{\begin{pmatrix} \underset{\text{Dx1}}{(x^{(1)})^\top} \\ (x^{(2)})^\top \\ \vdots \\ (x^{(N)})^\top \end{pmatrix}} \qquad Y = \underset{\text{Nx1}}{[y^{(1)}, y^{(2)}, \cdots, y^{(N)}]^\top}$$

  - Then $\underset{\text{NxD}}{\mathrm{RSS}(\theta)} = \underset{\text{Nx1}}{(X\theta - Y)^\top (X\theta - Y)}$

Empirical risk minimization

- Empirical risk for square loss:

$$\frac{1}{N}\sum_{n=1}^{N} L(y^{(n)}, h(x^{(n)})) = \frac{1}{N}\sum_{n=1}^{N}(y^{(n)} - h(x^{(n)}))^2$$

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Dx1

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NxD Dx1 Nx1

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Nx1

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Dx1

- Then $\underset{\text{Nx1}}{\text{RSS}(\theta)} = \underbrace{(X\theta - Y)^\top}_{\text{NxD Dx1}}\underbrace{(X\theta - Y)}_{\text{Nx1}}$

Empirical risk minimization

- Empirical risk for square loss:

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Dx1

$$Y = \underset{\text{Nx1}}{[y^{(1)}, y^{(2)}, \cdots, y^{(N)}]^\top}$$

- Then $\underset{\text{NxD}\ \ \text{Dx1}\ \ \text{Nx1}}{\text{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)}$

$\underbrace{\qquad}_{\text{1xN}}$ $\underbrace{\qquad}_{\text{Nx1}}$

Empirical risk minimization

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same objective from maximum likelihood! (up to a constant factor)

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- Notation:

$$Y = [y^{(1)}, y^{(2)}, \cdots, y^{(N)}]^\top$$

Nx1

$$X = \underset{\text{NxD}}{\begin{pmatrix} (x^{(1)})^\top \\ (x^{(2)})^\top \\ \vdots \\ (x^{(N)})^\top \end{pmatrix}}$$

Dx1

- Then $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$

NxD Dx1 Nx1

1xN Nx1

1x1

Let’s optimize!

Let’s optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$

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  - First-order conditions:

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  - First-order conditions: $\nabla \mathrm{RSS}(\theta) =$

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2X^\top (X\theta - Y)$

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2X^\top (X\theta - Y)$

check you can derive!

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2X^\top (X\theta - Y) \overset{\text{set}}{=} 0$

check you can derive!

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with dth element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (d,d') element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2X^\top (X\theta - Y) \overset{\text{set}}{=} 0$

check you can derive!

Dx1

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}(X\theta - Y) \overset{\text{set}}{=} 0$

check you can derive!

Dx1

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

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- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
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  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

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- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
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  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions:

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) =$

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2X^\top X$

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}}$

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- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
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  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}}$

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- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
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  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}} \overset{\text{set}}{>} 0$ is positive definite

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
  - The Hessian $\nabla^2_\theta f$ is the DxD matrix with (*d*,*d'*) element $\frac{\partial^2 f}{\partial \theta_d \partial \theta_{d'}}$
  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} 0$ (Dx1; Dx1)

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}} \overset{\text{set}}{>} 0$ (is positive definite)
  - For now, suppose *N*>*D* & *X* is full rank

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
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check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}} \overset{\text{set}}{>} 0$ is positive definite
- For now, suppose *N*>*D* & *X* is full rank
  - I.e. *X* has rank *D*, i.e. columns linearly independent

Let's optimize!

- We want to minimize $\mathrm{RSS}(\theta) = (X\theta - Y)^\top (X\theta - Y)$
  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
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  - First-order conditions: $\nabla \mathrm{RSS}(\theta) = 2\underbrace{X^\top}_{\text{DxN}}\underbrace{(X\theta - Y)}_{\text{Nx1}} \overset{\text{set}}{=} \underbrace{0}_{\text{Dx1}}$

check you can derive!

  - Second-order conditions: $\nabla^2 \mathrm{RSS}(\theta) = 2\underbrace{X^\top X}_{\text{DxD}} \overset{\text{set}}{>} 0$ is positive definite
- For now, suppose *N*>*D* & *X* is full rank
  - I.e. *X* has rank *D*, i.e. columns linearly independent
  - Then $X^\top X$ is positive definite and invertible

Let's optimize!

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  - Notation: for function $f(\theta)$, the gradient $\nabla_\theta f$ is the Dx1 vector with *d*th element: $\partial f / \partial \theta_d$
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"ordinary least squares" (OLS)

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- A closed-form solution isn't always better
  - Matrix inversion can be expensive for large dimensions

References (1/1)

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