Russ Salakhutdinov

9 October at 21:59 ·

I am teaching a Deep Learning graduate course this Fall at CMU with over 300 MSc and PhD students enrolled.

Today, after our midterm, I received the following anonymous feedback: "Did I take the wrong exam? Does this exam cover too little machine learning stuff and focus too much on mathematics?"

I guess there is a common belief that Deep Learning is all about installing TensorFlow or PyTorch and training a gigantic convnet on multiple GPUs 😃

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Csaba Szepesvari, Anima Anandkumar and 1.3k others

Outline

Goals

- Review the supervised learning setting
- Describe the linear regression framework
- Apply the linear model to make predictions
- Derive the least squares estimate

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Supervised Learning Setting

- Data consists of input and output pairs
- Inputs (also covariates, independent variables, predictors, features)
- Output (also variates, dependent variables, targets, labels)

Why study linear regression?

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- Often real processes can be approximated by linear models
- More complex models require understanding linear regression

- Closed form analytic solutions can be obtained
- Many key notions of machine learning can be introduced

A toy example : Commute Times

Want to predict commute time into city centre

What variables would be useful?

- Distance to city centre
- Day of the week

Data

dist (km)	day	commute time (min)
2.7	fri	25
4.1	mon	33
1.0	sun	15
5.2	tue	45
2.8	sat	22

Linear Models

Suppose the input is a vector $\mathbf{x} \in \mathbb{R}^D$ and the output is $y \in \mathbb{R}$.

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Notation: data dimension D, size of dataset N, column vectors

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Linear Model

$$y = w_0 + x_1 w_1 + \cdots + x_D w_D + \epsilon$$

Bias/intercept

Noise/uncertainty

Linear Models : Commute Time

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- monday: 0, tuesday: 1, . . . , sunday: 6
- 0 if weekend, 1 if weekday

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Say $x_1 \in \mathbb{R}$ (distance) and $x_2 \in \{0, 1\}$ (weekend/weekday)

Linear model for commute time

$$y = w_0 + w_1 x_1 + w_2 x_2 + \epsilon$$

Linear Model : Adding a feature for bias term

dist	day	commute time
x_1	x_2	y
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Model

$$y = w_0 + w_1 x_1 + w_2 x_2 + \epsilon$$

Model

$$\begin{aligned} y &= w_0 x_0 + w_1 x_1 + w_2 x_2 + \epsilon \\ &= \mathbf{w} \cdot \mathbf{x} + \epsilon \end{aligned}$$

Learning Linear Models

Data: $\langle(\mathbf{x}_i, y_i)\rangle_{i=1}^{N}$, where $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \mathbb{R}$

Model parameter $\mathbf{w}$, where $\mathbf{w} \in \mathbb{R}^D$

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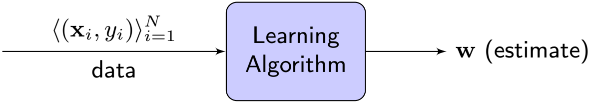

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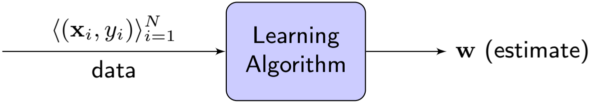

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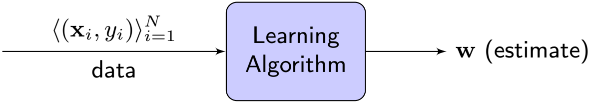

Testing/Deployment phase: (predict $\widehat{y}_{\text{new}} = \mathbf{x}_{\text{new}} \cdot \mathbf{w}$)

- How different is $\widehat{y}_{\text{new}}$ from y_{new} (actual observation)?
- We should keep some data aside for testing before deploying a model

$\langle (x_i, y_i) \rangle_{i=1}^{N}$, where $x_i \in \mathbb{R}$ and $y_i \in \mathbb{R}$

$\widehat{y}(x) = w_0 + x \cdot w_1$, (no noise term in $\widehat{y}$)

$$\mathcal{L}(\mathbf{w}) = \mathcal{L}(w_0, w_1) = \frac{1}{2N} \sum_{i=1}^{N} (\widehat{y_i} - y_i)^2 = \frac{1}{2N} \sum_{i=1}^{N} (w_0 + x_i \cdot w_1 - y_i)^2$$

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Energy Function
Notation - $\mathcal{L}, J, E, R$

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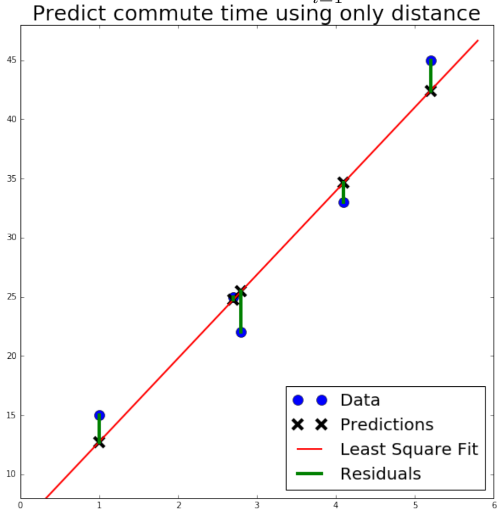

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This objective is known as the residual sum of squares or (RSS)

The estimate (w_0, w_1) is known as the least squares estimate

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We obtain the solution for (w_0, w_1) by setting the partial derivatives to 0 and solving the resulting system. (Normal Equations)

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$$\bar{y} = \frac{\sum_i y_i}{N}$$

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$$w_1 = \frac{\widehat{\mathrm{cov}}(x, y)}{\widehat{\mathrm{var}}(x)}$$

$$w_0 = \bar{y} - w_1 \cdot \bar{x}$$

Linear Regression : General Case

Recall that the linear model is

$$\widehat{y}_i = \sum_{j=0}^{D} x_{ij} w_j$$

where we assume that $x_{i0} = 1$ for all $\mathbf{x}_i$, so that the bias term w_0 does not need to be treated separately.

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Expressing everything in matrix notation

$$\widehat{\mathbf{y}} = \mathbf{X}\mathbf{w}$$

Here we have $\widehat{\mathbf{y}} \in \mathbb{R}^{N\times 1}$, $\mathbf{X} \in \mathbb{R}^{N\times(D+1)}$ and $\mathbf{w} \in \mathbb{R}^{(D+1)\times 1}$

$$\overset{\widehat{\mathbf{y}}_{N\times 1}}{\begin{bmatrix} \widehat{y}_1 \\ \widehat{y}_2 \\ \vdots \\ \widehat{y}_N \end{bmatrix}} = \overset{\mathbf{X}_{N\times(D+1)}}{\begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix}} \overset{\mathbf{w}_{(D+1)\times 1}}{\begin{bmatrix} w_0 \\ \vdots \\ w_D \end{bmatrix}} = \overset{\mathbf{X}_{N\times(D+1)}}{\begin{bmatrix} x_{10} & \cdots & x_{1D} \\ x_{20} & \cdots & x_{2D} \\ \vdots & \ddots & \vdots \\ x_{N0} & \cdots & x_{ND} \end{bmatrix}} \overset{\mathbf{w}_{(D+1)\times 1}}{\begin{bmatrix} w_0 \\ \vdots \\ w_D \end{bmatrix}}$$

Back to toy example

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We have $N = 5$, $D + 1 = 3$ and so we get

$$\mathbf{y} = \begin{bmatrix} 25 \\ 33 \\ 15 \\ 45 \\ 22 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & 2.7 & 1 \\ 1 & 4.1 & 1 \\ 1 & 1.0 & 0 \\ 1 & 5.2 & 1 \\ 1 & 2.8 & 0 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$$

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Suppose we get $\mathbf{w} = [6.09, 6.53, 2.11]^{\mathsf{T}}$. Then our predictions would be

$$\widehat{\mathbf{y}} = \begin{bmatrix} 25.83 \\ 34.97 \\ 12.62 \\ 42.16 \\ 24.37 \end{bmatrix}$$

Least Squares Estimate : Minimise the Squared Error

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{x}_i^{\mathsf{T}}\mathbf{w} - y_i)^2 = \frac{1}{2N}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^{\mathsf{T}}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)$$

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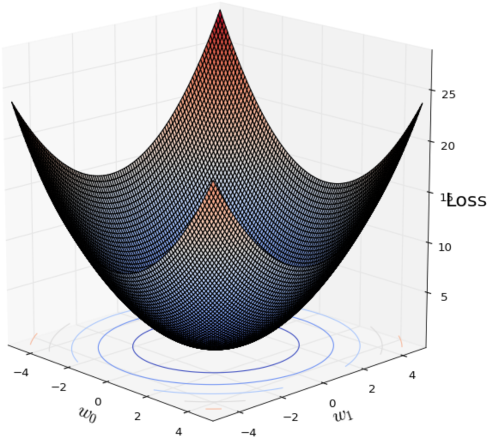

Finding Optimal Solutions using Calculus

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$$= \frac{1}{2N}\left(\mathbf{w}^{\mathsf{T}}\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)\mathbf{w} - \mathbf{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{y} - \mathbf{y}^{\mathsf{T}}\mathbf{X}\mathbf{w} + \mathbf{y}^{\mathsf{T}}\mathbf{y}\right)$$

Finding Optimal Solutions using Calculus

$$
\begin{aligned}
\mathcal{L}(\mathbf{w}) &= \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2 = \frac{1}{2N}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^\top \left(\mathbf{X}\mathbf{w} - \mathbf{y}\right) \\
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&= \cdots
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Then, write out all partial derivatives to form the gradient $\nabla_{\mathbf{w}}\mathcal{L}$

Finding Optimal Solutions using Calculus

$$\begin{aligned}
\mathcal{L}(\mathbf{w}) &= \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{x}_i^\mathsf{T}\mathbf{w} - y_i)^2 = \frac{1}{2N}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^\mathsf{T}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right) \\
&= \frac{1}{2N}\left(\mathbf{w}^\mathsf{T}\left(\mathbf{X}^\mathsf{T}\mathbf{X}\right)\mathbf{w} - \mathbf{w}^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{y} - \mathbf{y}^\mathsf{T}\mathbf{X}\mathbf{w} + \mathbf{y}^\mathsf{T}\mathbf{y}\right) \\
&= \frac{1}{2N}\left(\mathbf{w}^\mathsf{T}\left(\mathbf{X}^\mathsf{T}\mathbf{X}\right)\mathbf{w} - 2\cdot\mathbf{y}^\mathsf{T}\mathbf{X}\mathbf{w} + \mathbf{y}^\mathsf{T}\mathbf{y}\right) \\
&= \cdots
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\frac{\partial\mathcal{L}}{\partial w_0} &= \cdots \\
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&\vdots \\
\frac{\partial\mathcal{L}}{\partial w_D} &= \cdots
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Finding Optimal Solutions using Calculus

$$
\begin{aligned}
\mathcal{L}(\mathbf{w}) &= \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2 = \frac{1}{2N}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^\top \left(\mathbf{X}\mathbf{w} - \mathbf{y}\right) \\
&= \frac{1}{2N}\left(\mathbf{w}^\top \left(\mathbf{X}^\top \mathbf{X}\right)\mathbf{w} - \mathbf{w}^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\mathbf{w} + \mathbf{y}^\top \mathbf{y}\right) \\
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&\vdots \\
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\end{aligned}
$$

Instead, we will use matrix calculus shortcuts to differentiate using matrix notation directly

Differentiating Matrix Expressions

Rules (Tricks)

(i) Linear Form Expressions: $\nabla_{\mathbf{w}} \left(\mathbf{c}^{\mathsf{T}} \mathbf{w} \right) = \mathbf{c}$

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$$\frac{\partial \left(\mathbf{c}^{\mathsf{T}} \mathbf{w} \right)}{\partial w_j} = c_j, \qquad \text{and so} \qquad \nabla_{\mathbf{w}} \left(\mathbf{c}^{\mathsf{T}} \mathbf{w} \right) = \mathbf{c} \tag{3}$$

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$$\mathbf{w}^{\mathsf{T}} \mathbf{A} \mathbf{w} = \sum_{i=0}^{D} \sum_{j=0}^{D} w_i w_j A_{ij}$$

$$\frac{\partial \left(\mathbf{w}^{\mathsf{T}} \mathbf{A} \mathbf{w} \right)}{\partial w_k} = \sum_{i=0}^{D} w_i A_{ik} + \sum_{j=0}^{D} A_{kj} w_j = \mathbf{A}_{[:,k]}^{\mathsf{T}} \mathbf{w} + \mathbf{A}_{[k,:]} \mathbf{w}$$

$$\nabla_{\mathbf{w}} \left(\mathbf{w}^{\mathsf{T}} \mathbf{A} \mathbf{w} \right) = \mathbf{A}^{\mathsf{T}} \mathbf{w} + \mathbf{A} \mathbf{w} \tag{4}$$

Deriving the Least Squares Estimate

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{x}_i^\mathsf{T}\mathbf{w} - y_i)^2 = \frac{1}{2N}\left(\mathbf{w}^\mathsf{T}\left(\mathbf{X}^\mathsf{T}\mathbf{X}\right)\mathbf{w} - 2\cdot\mathbf{y}^\mathsf{T}\mathbf{X}\mathbf{w} + \mathbf{y}^\mathsf{T}\mathbf{y}\right)$$

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$$\left(\mathbf{X}^\top \mathbf{X} \right) \mathbf{w} = \mathbf{X}^\top \mathbf{y}$$

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The predictions made by the model on the data $\mathbf{X}$ are given by

$$\widehat{\mathbf{y}} = \mathbf{X}\mathbf{w} = \mathbf{X}\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y}$$

For this reason the matrix $\mathbf{X}\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}$ is called the “hat” matrix

Least Squares Estimate

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  We always have $x_{\mathrm{mon}} + \cdots + x_{\mathrm{sun}} = 1$

  This introduces a linear dependence in the columns of $\mathbf{X}$ reducing the rank

  In this case, we can drop some features to adjust rank. We'll see alternative approaches later in the course.

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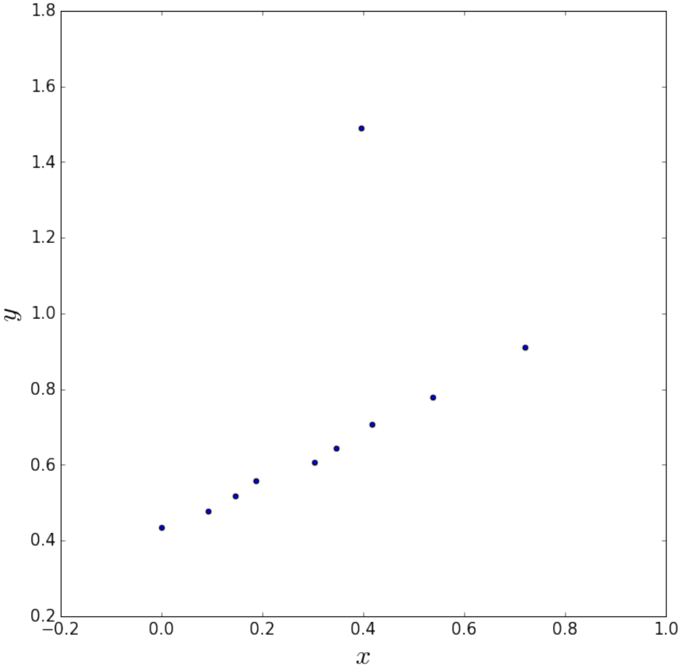
  Relatively easy to get $O(D^2 N)$ bound


1.8
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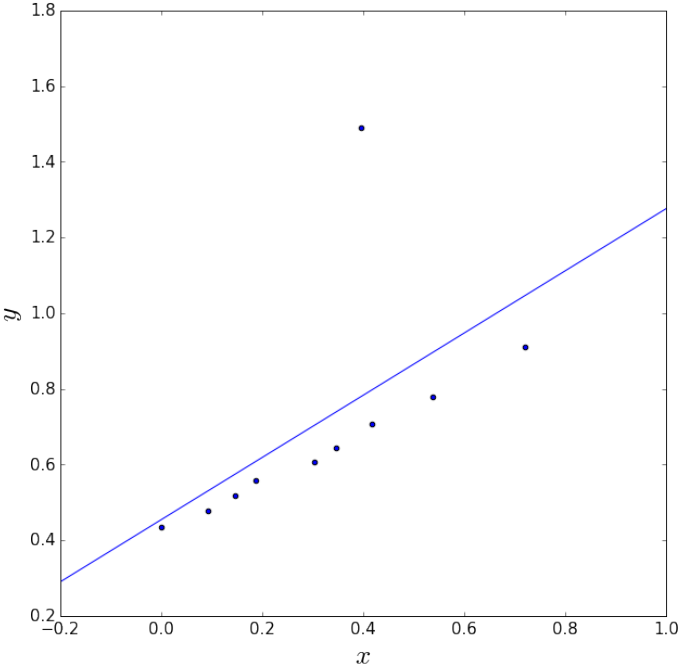
x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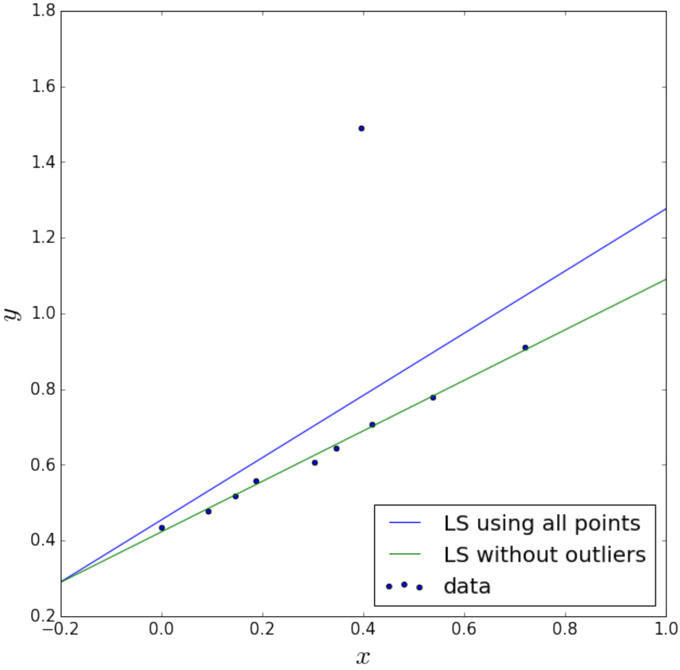

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y
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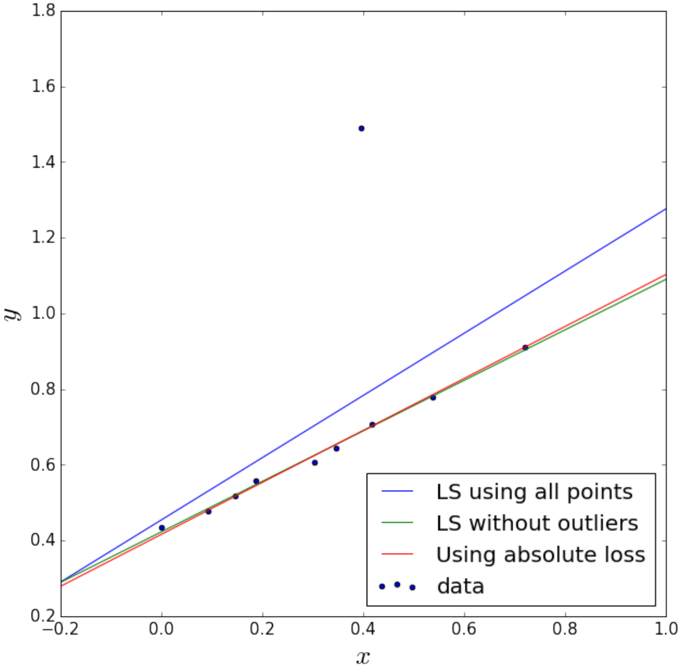
LS using all points
LS without outliers
data



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Using absolute loss
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Recap : Predicting Commute Time

Goal

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- Predict the time taken for commute given distance and day of week

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Model and Choice of Loss Function

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Model and Choice of Loss Function

- Use a linear model

$$y = w_0 + w_1 x_1 + \cdots + w_D x_D + \epsilon = \widehat{y} + \epsilon$$

- Minimise average squared error $\frac{1}{2N} \sum (y_i - \widehat{y_i})^2$

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Algorithm to Fit Model

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Algorithm to Fit Model

- Simple matrix operations using closed-form solution

Model and Loss Function Choice

"Optimisation" View of Machine Learning

- Pick model that you expect may fit the data well enough
- Pick a measure of performance that makes "sense" and can be optimised
- Run optimisation algorithm to obtain model parameters

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Probabilistic View of Machine Learning

- Pick a model for data and explicitly formulate the deviation (or uncertainty) from the model using the language of probability
- Use notions from probability to define suitability of various models
- "Find" the parameters or make predictions on unseen data using these suitability criteria (Frequentist vs Bayesian viewpoints)