Linear Mean Functions and Ordinary Least Squares

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Computational Methods in Statistics and Data Science (Stats 406)

Smoothed Means

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- Trade-off in the size of the bandwidth with respect to bias and variance
- Used bootstrapping to get confidence intervals.

Mean Functions for Multiple x

Multivariate Smoothing

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In principle, we could **plug these into the Nadaraya-Watson estimator**.

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The Curse of Dimensionality: as the number of dimensions increases all points are far apart.

Illustration

Suppose $x_j \in [0, 1]$ for $j = 1, \ldots, p$. Consider the point

$$\mathbf{x} = (0.5, 0.5, \ldots, 0.5)^T$$

(notation: $\mathbf{x}$ is a column vector of size p)

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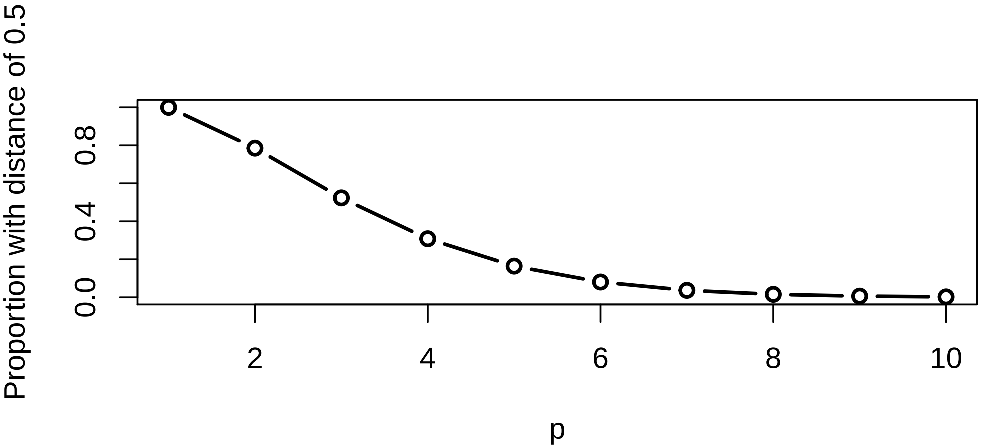
What proportion of the points in the space are within a distance of 0.5 of x?

$$\frac{\text{volume of a sphere of radius 0.5}}{\text{volume of a } p\text{-dimensional box}} = \frac{\pi^{p/2}}{p 2^{p-1} \Gamma(p/2)}$$



Proportion with distance of 0.5
0.0
0.4
0.8
2
4
6
8
10
p

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- Smoothing estimators require evaluating an expression **at each point of the original data** (no data compression).
- We want to **include additional structure**.
- We want to interpret the **contribution of** x_j apart from the other predictors.

Solution

We'll consider a variety of methods that address the problems using these steps:

- **Reduce the dimension** from p to 1 using a function $\eta(x_1, \dots, x_p; \beta)$ and a parameter β

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Compared to other statistics courses our emphasis will be on β as a **solution to an optimization problem** (i.e., minimizing loss).

Ordinary Least Squares

Vector and Matrix Notation

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Note: we think of y as random, but I'm writing it as lower case now that we have to deal with vectors and matrices.

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$$\mathbf{a}^T\mathbf{b} = \sum_{i=1}^{n} a_i b_i$$

A very quick linear algebra review

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For matrices $\mathbf{A}$ ($n \times p$) and $\mathbf{B}$ ($p \times m$), the matrix $\mathbf{AB} = \mathbf{C}$ ($n \times m$) has entries:

$$c_{ij} = (i\text{th row of } \mathbf{A})^T (j\text{th column of } \mathbf{B})$$

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If a matrix $\mathbf{A}$ is square $(n \times n)$ and the columns are linearly independent ("full rank"), then the **matrix inverse** $\mathbf{A}^{-1}$ is such that

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}_n$$

where $\mathbf{I}_n$ is the **identity matrix**, with 1's on the diagonal and 0's elsewhere.

Simplest μ and η

Recall that we are modeling:

$$y = \mu(\eta(\mathbf{x}; \boldsymbol{\beta})) + \epsilon, \quad \text{where } \boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)^T$$

(semi-colon notation indicates that while $\mathbf{x}$ will change for different observations, $\boldsymbol{\beta}$ will be the same – e.g. likelihoods)

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First, we need a function η that maps our observations $\mathbf{x}$ to a scalar. The probably the simplest such function:

$$\eta(\mathbf{x}; \boldsymbol{\beta}) = \mathbf{x}^T \boldsymbol{\beta} = \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p$$

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Next, we need a function μ that maps scalars to scalars. The simplest function:

$$\mu(a) = a$$

Putting them together

Combining μ and η, we arrive at **a model for the mean function**:

$$\mathrm{E}\left(y \mid \mathbf{x}\right) = \mu(\eta(\mathbf{x}; \boldsymbol{\beta})) = \mathbf{x}^T \boldsymbol{\beta}$$

or equivalently

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NB: We often set $x_0 = 1$ for all units so p includes $p - 1$ "real variables":

$$y = \beta_0 + \beta_1 x_1 + \ldots \beta_{p-1} x_{p-1} + \epsilon$$

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Both are examples of **convex loss functions**, which means that any **local optimum** is also the **global optimum**.

One dimensional case

Let's simulate an outcome that is **linear in** x, $\mathbf{E}(\epsilon = 0)$, but **does not follow usual Normal assumptions**:

$$x \sim U(0, 100)$$

$$\epsilon \sim 0.25N\left(1, 2(x-50)^2 + 10\right) + 0.75N\left(-1/3, 2(x-50)^2 + 10\right)$$

$$y = 3x + \epsilon$$

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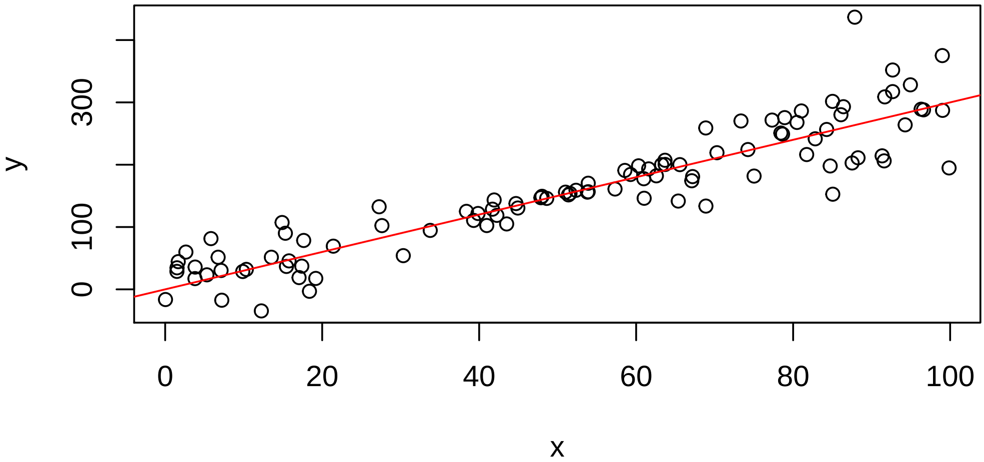
```
> n <- 100
> x <- runif(n, 0, 100)
> epsilon <- rnorm(n,
+                  mean = 1 - 4/3 * rbinom(n, size = 1, prob = 0.75),
+                  sd = sqrt(2 * abs(x - 50)^2 + 10))
> y <- 3 * x + epsilon
```



0
100
300
y
0
20
40
60
80
100
x

Loss functions

```
> loss_abs <- function(beta) {
+     sum(abs(y - beta * x))
+ }
> loss_sqd <- function(beta) {
+     sum((y - beta * x)^2)
+ }
```

Brute Force Solutions

```
> betas <- seq(-10, 10, length.out = 1000)
> beta_loss_abs <- map_dbl(betas, loss_abs)
> beta_loss_sqd <- map_dbl(betas, loss_sqd)
```

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> betas <- seq(-10, 10, length.out = 1000)
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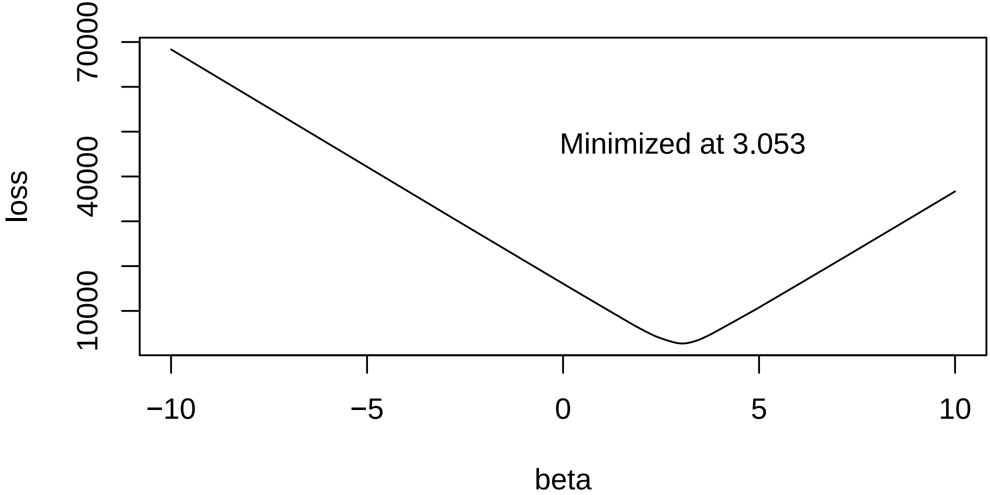
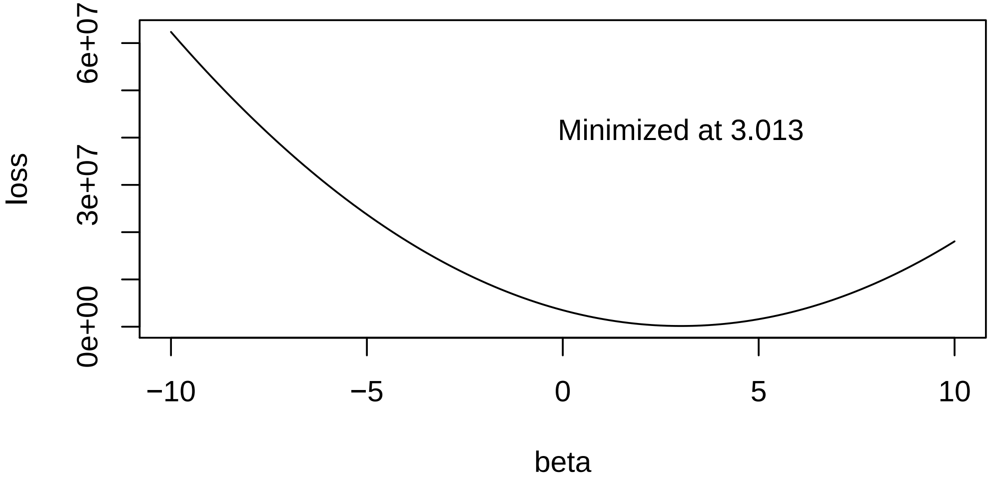
> best_abs <- betas[which.min(beta_loss_abs)]
> best_sqd <- betas[which.min(beta_loss_sqd)]
```

Plotting Absolute Loss



Plotting Squared Loss



Brute force depends on the grid

```
> betas_coarse <- seq(-10, 10, length.out = 10)
> betas_coarse[which.min(map_dbl(betas_coarse, loss_abs))] # Absolute Loss

[1] 3.333

> betas_coarse[which.min(map_dbl(betas_coarse, loss_sqd))] # Squared Loss

[1] 3.333
```

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We'll look at squared error loss today. We'll return to absolute loss with more advanced techniques.

Finding minimum for squared error loss

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&= \sum_{i=1}^{n} -2 \left(y_i - \mathbf{x_i}^T \boldsymbol{\beta} \right) x_{ij} \\
&= 2 \left[\sum_{i=1}^{n} \mathbf{x_i}^T \boldsymbol{\beta} \, x_{ij} - \sum_{i=1}^{n} y_i x_{ij} \right]
\end{aligned}$$

Expressing as a system of equations

We are seeking solutions $\hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_p$ such that

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We can stack the **system of p linear equations**:

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}$$

Where $\mathbf{X}$ is the $n \times p$ **design matrix** of stacked $\mathbf{x_i}$ vectors and $\mathbf{y}$ is the vector of outcomes

Solving systems of linear equations: Ordinary Least Squares

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$$\hat{\beta} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

But **computing matrix inverses** can be **numerically unstable**.

We are better off using techniques from your linear algebra course (**Gaussian elimination**!).

Luckily for us, R will handle actually computing solution:

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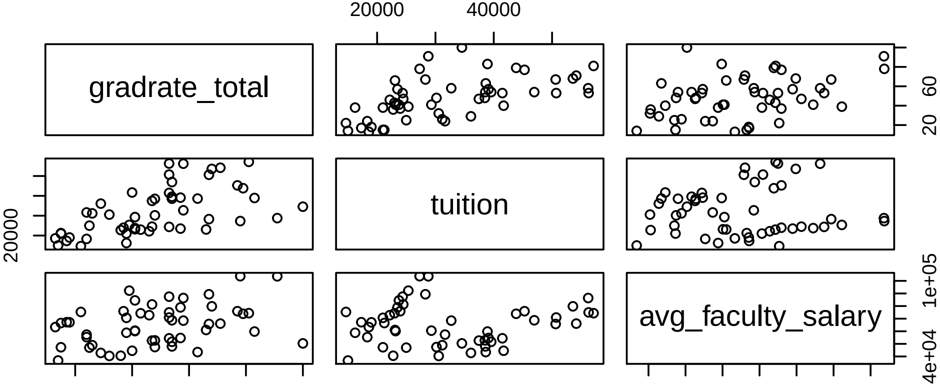
We call this solution, **ordinary least squares** because it minimized **squared error loss**.

Example: Graduation Rates

How do graduation of Michigan colleges and universities vary as a function of tuition and faculty salaries? (2016 data)



```
> edu_analysis[edu_analysis$name == "University of Michigan-Ann Arbor", 2:4

    gradrate_total tuition avg_faculty_salary
165             91   28776             103605

> design_matrix <- as.matrix(
+     cbind(1,
+           edu_analysis[, c("tuition", "avg_faculty_salary")]))
```

```
> XtX <- t(design_matrix) %*% design_matrix
> XtY <- t(design_matrix) %*% edu_analysis$gradrate_total
> (beta_hat <- as.vector(solve(XtX, XtY)))

[1] -1.426e+01  1.010e-03  4.583e-04
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> (mod <- lm(gradrate_total ~ tuition + avg_faculty_salary,
+             data = edu_analysis))

Call:
lm(formula = gradrate_total ~ tuition + avg_faculty_salary, data = edu_anal

Coefficients:
       (Intercept)             tuition  avg_faculty_salary
         -1.43e+01            1.01e-03            4.58e-04
```

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Note: be careful about scale! The units of the x variables are usually not the same, so **magnitude does not mean importance**!

Changes in Grad Rate (as percentage)

From the previous slides we see that **schools that differ by $1,000 tuition** differ by

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> 1000 * beta_hat[2]
```

```
[1] 1.01
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In both cases, **according to our model** and **holding all other variables equal**.

Inference

Recall our basic model for the (random) y:

$$y = \mu(\eta(\mathbf{x}; \boldsymbol{\beta}) + \epsilon = \mathbf{x}^T \boldsymbol{\beta} + \epsilon, \quad \mathsf{E}\left(\epsilon\right) = 0$$

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- Assume ϵ follow a specific distribution and sample from that to create $y^* = \mathbf{x}^T\hat{\boldsymbol{\beta}} + \epsilon^*$

Gaussian model for ϵ

If we assumed $\epsilon \sim N(0, \sigma^2)$ in

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then the **likelihood** of the data (with respect to $\boldsymbol{\beta}$ and assuming IID) would be:

$$L(\boldsymbol{\beta}) = f(y_1, \ldots, y_n; \boldsymbol{\beta}) = \frac{1}{\sqrt{2\pi\sigma^2}^n} \exp\left\{-\frac{\sum_{i=1}^n (y_i - \mathbf{x}_i^T\boldsymbol{\beta})^2}{2\sigma^2}\right\}$$

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And the **log-likelihood** is

$$l(\boldsymbol{\beta}) = n \log(\sqrt{2\pi\sigma^2}) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2$$

MLE of β for Gaussian Model

To find **maximum likelihood estimates**, we want to **maximize the log-likelihood**:

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The **squared error loss function**!

Not only is $\hat{\boldsymbol{\beta}}$ the solution to squared error loss, but is also **the maximum likelihood estimate** when under the Gaussian model.

Additional Implications of Gaussian Model

Our MLE estimate is the solution to

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This also implies a distribution for $\hat{\beta}$:

$$\hat{\beta} \sim N_p\left(\beta, \sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\right)$$

which can be used for tests and intervals.

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NB: Even if ϵ is not Normal, since $\hat{\boldsymbol{\beta}}$ is based on sample averages, the **central limit theorem** can also be used to justify these intervals.

```
> summary(mod)

Call:
lm(formula = gradrate_total ~ tuition + avg_faculty_salary, data = edu_analysis)

Residuals:
   Min     1Q Median     3Q    Max 
-24.10 -11.20  -0.71   8.05  56.27 

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)    
(Intercept)        -1.43e+01   1.07e+01   -1.33   0.1898    
tuition             1.01e-03   1.85e-04    5.47  1.5e-06 ***
avg_faculty_salary  4.58e-04   1.38e-04    3.33   0.0017 ** 
---
Signif. codes:  0
```

Adding constraints: Quadratic Programs

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Quadratic programs are those that can be specified as

$$\text{minimize:} \frac{1}{2}\boldsymbol{\beta}^T \mathbf{D}\boldsymbol{\beta} - \mathbf{c}^T\boldsymbol{\beta} \quad \text{(with respect to } \boldsymbol{\beta}\text{)}$$

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OLS is a **special case** of a quadratic program.

OLS as QP

$$\sum_{i=1}^{n}(y_i - \boldsymbol{\beta}^T \mathbf{x}_i)^2 = \sum_{i=1}^{n} y_i^2 - 2\boldsymbol{\beta}^T \mathbf{x}_i y_i + (\boldsymbol{\beta}^T \mathbf{x}_i)^2$$

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$$\approx \sum_{i=1}^{n}(\boldsymbol{\beta}^T \mathbf{x}_i)(\mathbf{x}_i^T \boldsymbol{\beta}) - 2\boldsymbol{\beta}^T \mathbf{x}_i y_i$$

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\begin{aligned}
\sum_{i=1}^{n} (y_i - \boldsymbol{\beta}^T \mathbf{x}_i)^2 &= \sum_{i=1}^{n} y_i^2 - 2\boldsymbol{\beta}^T \mathbf{x}_i y_i + (\boldsymbol{\beta}^T \mathbf{x}_i)^2 \\
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&= \boldsymbol{\beta}^T \left[\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T \right] \boldsymbol{\beta} - 2\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y}
\end{aligned}
$$

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&= \boldsymbol{\beta}^T \left[\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T \right] \boldsymbol{\beta} - 2\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} \\
&\propto \frac{1}{2} \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X} \boldsymbol{\beta} - (\mathbf{X}^T \mathbf{y})^T \boldsymbol{\beta}
\end{aligned}
$$

Non-negative least squares in R

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$$\mathbf{I}_p \boldsymbol{\beta} \geq \mathbf{0}$$

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> library(quadprog)
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In the previous (unconstrained) OLS fit, we got a negative intercept, now we forced it to be non-negative.

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- Found that **squared error loss** can be solved using a **system of linear equations** (easy!)
- Considered how to **interpret** and **add uncertainty** to estimates.
- Used the optimization perspective to add constraints.