

T04: Outliers and l_1 loss

MATH 4432 Statistical Machine Learning

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Let's start by recalling linear
regression!

Least squares

Recall the least squares (LS) problem for linear regression

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^N (y_i - x_i \beta)^2 = \underset{\beta}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N (y_i - x_i \beta)^2.$$

A toy example

Code

Minimize the squared loss

- Suppose we know the ground truth of $f(\cdot) : f(x) = x$
- Now given $\{x_i\}_{i=1}^N$, we have a set of observations $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ with

$$y_i = f(x_i) + \epsilon_i,$$

where $\epsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 0.1^2)$ is random noise.

Least squares

Recall the least squares (LS) problem for linear regression

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^N (y_i - x_i \beta)^2 = \underset{\beta}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N (y_i - x_i \beta)^2.$$

A toy example

Code

Minimize the squared loss

```
set.seed(123)
N <- 10 # Sample size
x <- runif(N, 0, 1)
y0 <- x # Ground truth
y_obs <- y0 + rnorm(N, mean = 0, sd = 0.1) # Add noise, observed data
ggplot(data = NULL, aes(x = x, y = y_obs)) +
  geom_point(aes(x = x, y = y_obs), size = 5) +
  geom_smooth(method = "lm", size = 1.5) +
  theme(
    text = element_text(size = 18),
    axis.text.y = element_text(size = 18),
    axis.text.x = element_text(size = 18)
  )
```

Least squares

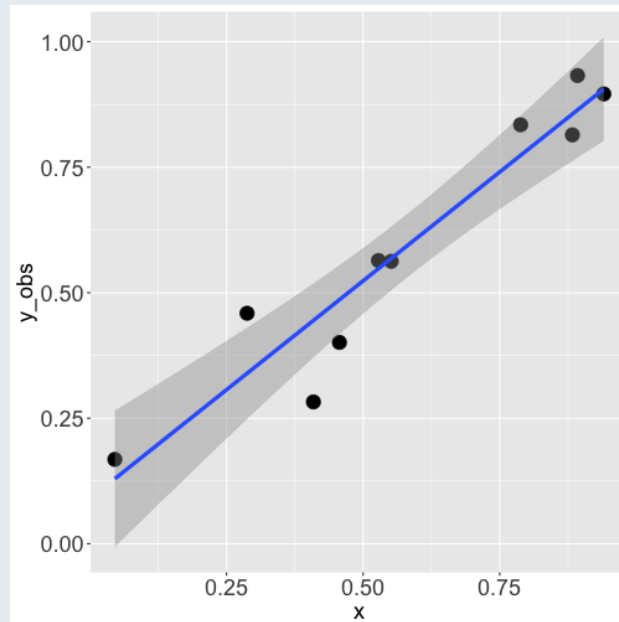
Recall the least squares (LS) problem for linear regression

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^N (y_i - x_i \beta)^2 = \underset{\beta}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N (y_i - x_i \beta)^2.$$

A toy example

Code

Minimize the squared loss



What if there exists an outlier?

Add an outlier

Add an outlier

Code

Minimize the squared loss

- We follow the above problem setting.
- But add an outlier

$$(x, y, y_{\text{obs}}) = (0.9, 0.9, -2),$$

of which the noise is extremely large. This situation is rare, but the probability is not zero!

Add an outlier

Add an outlier

Code

Minimize the squared loss

```
set.seed(123)

x_ol <- c(x, 0.9)
y0_ol <- c(y0, 0.9)
y_obs_ol <- c(y_obs, -2) # Add noise, observed data

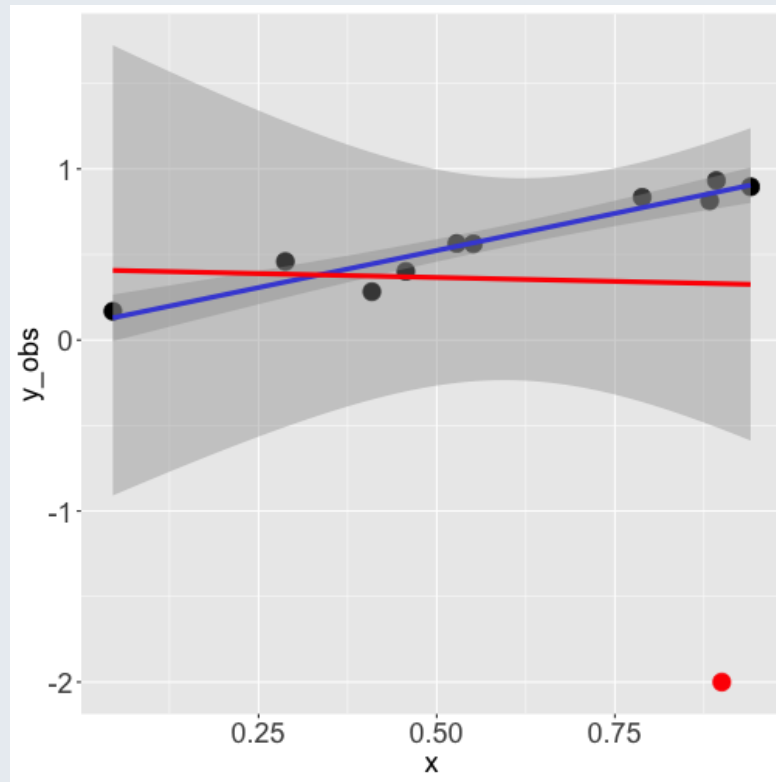
ggplot(data = NULL) +
  geom_point(aes(x = x, y = y_obs), size = 5) +
  geom_point(aes(x = 0.9, y = -2), color = "red", size = 5) +
  geom_smooth(aes(x = x, y = y_obs), method = "lm", color = "blue", size = 2) +
  geom_smooth(aes(x = x_ol, y = y_obs_ol), method = "lm", color = "red", size = 2) +
  theme(
    text = element_text(size = 18),
    axis.text.y = element_text(size = 18),
    axis.text.x = element_text(size = 18)
  )
```


Add an outlier

Add an outlier

Code

Minimize the squared loss



Brief summary of squared loss

Pros

- Natural, intuitive (Euclidean distance)
- Closed form solution

Con

- Not robust to outliers, equal weights to all data (assumes Gaussian distributed residual)

Let's consider a more robust loss
function!

l_1 loss

- l_2 norm and l_1 norm

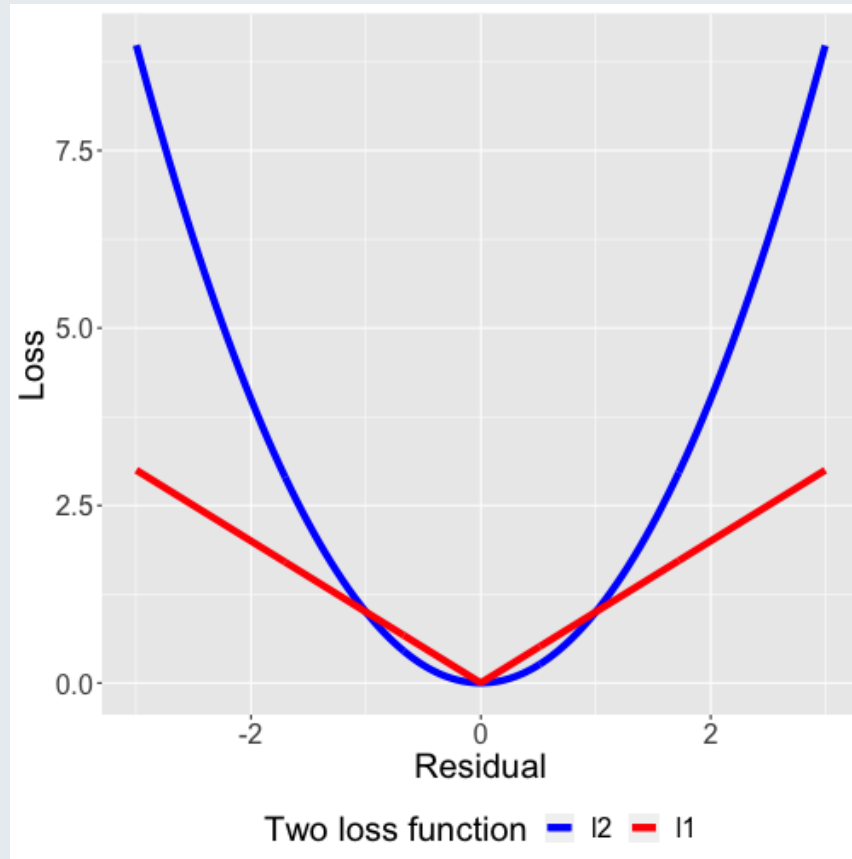
$$||x||_2 = \left(\sum_{j=1}^p x_j^2 \right)^{\frac{1}{2}}, \quad ||x||_1 = \sum_{j=1}^p |x_j|.$$

- l_2 loss and l_1 loss

$$\mathcal{L}_2 = \sum_{i=1}^N (y_i - x_i \beta)^2 = ||y - X\beta||_2^2,$$

$$\mathcal{L}_1 = \sum_{i=1}^N |y_i - x_i \beta| = ||y - X\beta||_1.$$

Why is l_1 more robust?



However, the bad news is that l_1 loss function is not differentiable :(

Let's relax it!

MM algorithm *

The "MM" stands for "Majorization-Minimization" or "Minorization-Maximization". In the following "MM" refers to "Majorization-Minimization".

- Consider the following presumably difficult optimization problem

$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} \ f(\mathbf{x}) \\ & \text{subject to } \mathbf{x} \in \mathcal{X}, \end{aligned}$$

with \mathcal{X} being the feasible set and $f(\mathbf{x})$ being continuous.

- Idea: successively minimize a more manageable surrogate function $u(\mathbf{x}, \mathbf{x}^k)$

$$\mathbf{x}^{k+1} = \arg \min_{\mathbf{x} \in \mathcal{X}} u(\mathbf{x}, \mathbf{x}^k),$$

hoping the sequence of minimizers $\{\mathbf{x}^k\}$ will converge to optimal \mathbf{x}^* .

[*] Not required in this course. Materials are from ELEC 5470 / IEDA 6100A Convex Optimization, Prof. Daniel P. Palomar, ECE, HKUST.

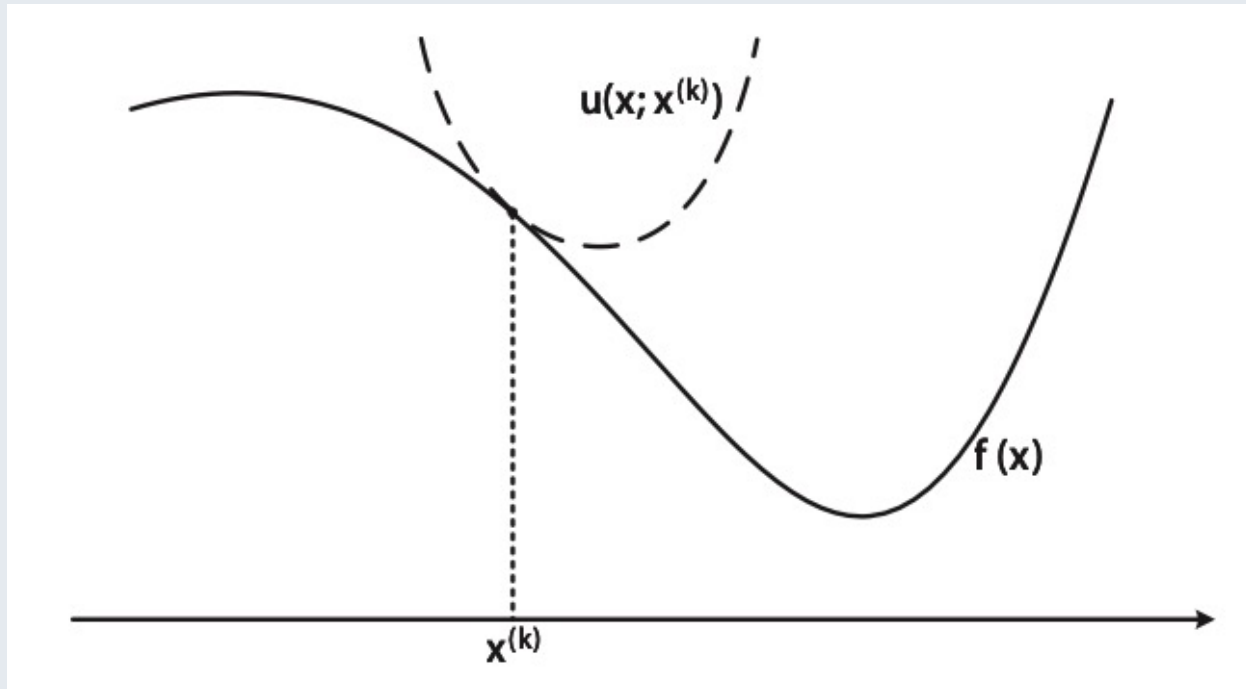
Iterative algorithm

Suppose x_0 is the initial point, in k -th step, we want $x_{k-1} \rightarrow x_k$.

After k -th step

($k+1$)-th step

($k+2$)-th step



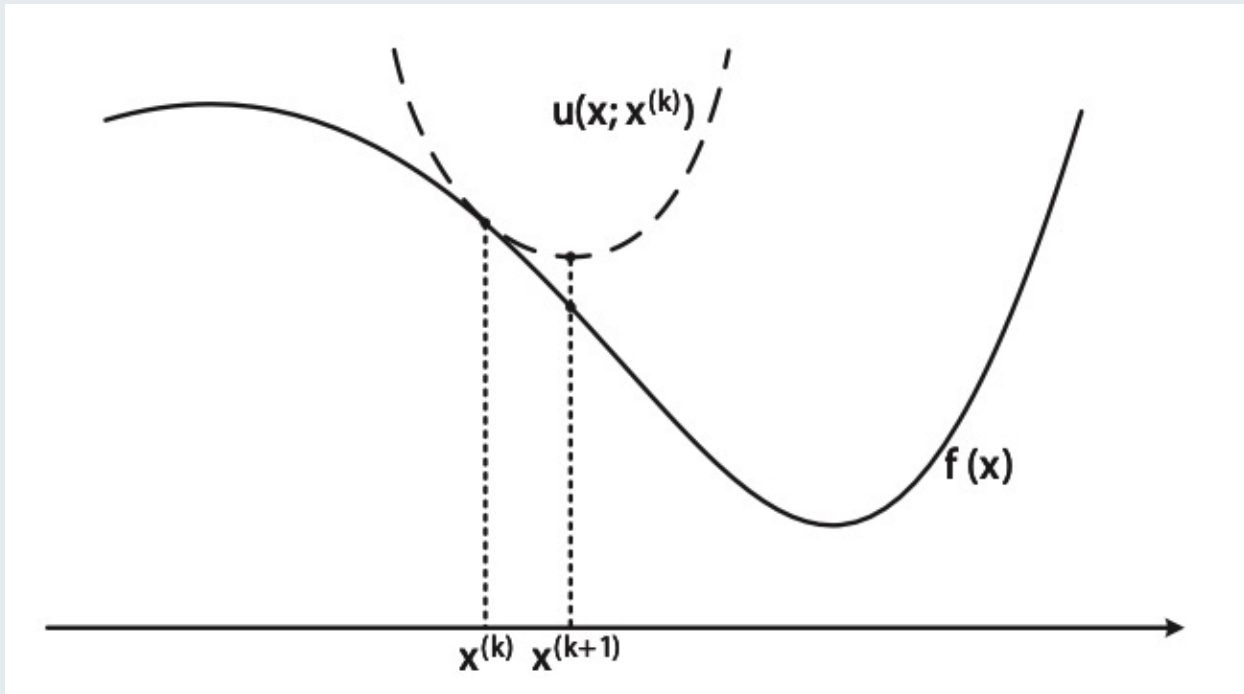
Iterative algorithm

Suppose x_0 is the initial point, in k -th step, we want $x_{k-1} \rightarrow x_k$.

After k -th step

($k+1$)-th step

($k+2$)-th step



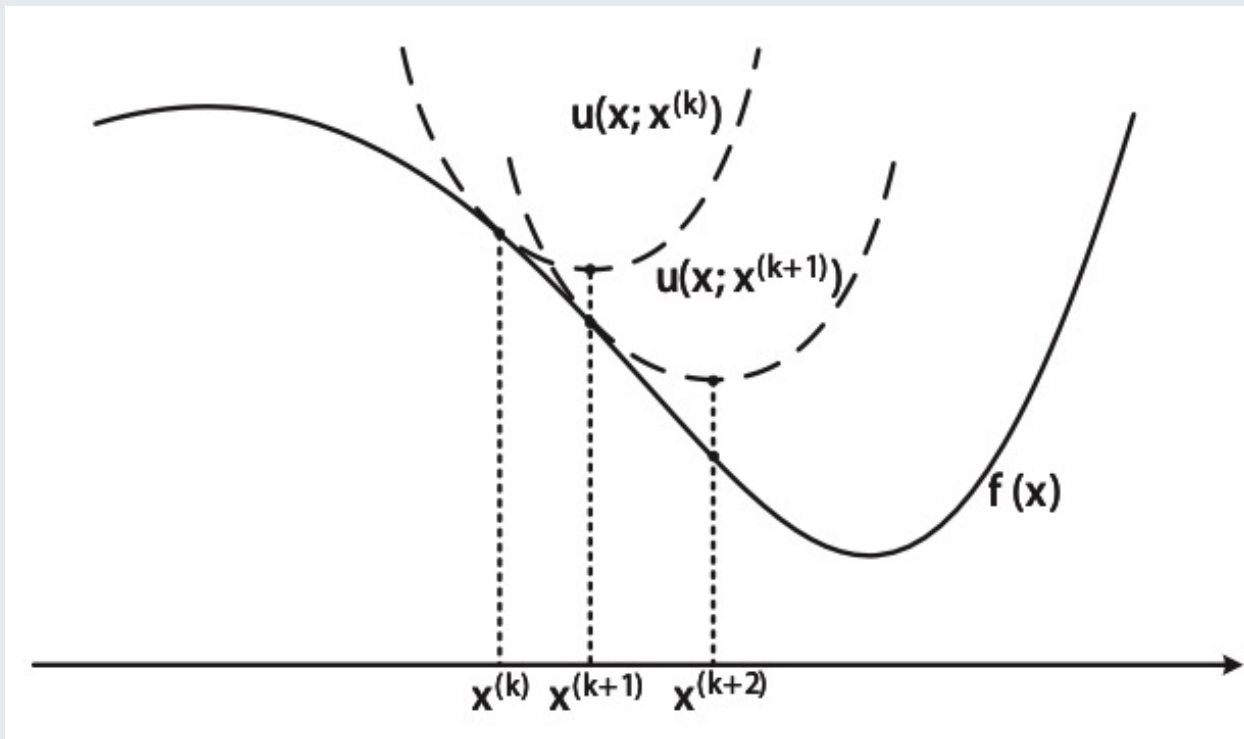
Iterative algorithm

Suppose x_0 is the initial point, in k -th step, we want $x_{k-1} \rightarrow x_k$.

After k -th step

$(k+1)$ -th step

$(k+2)$ -th step



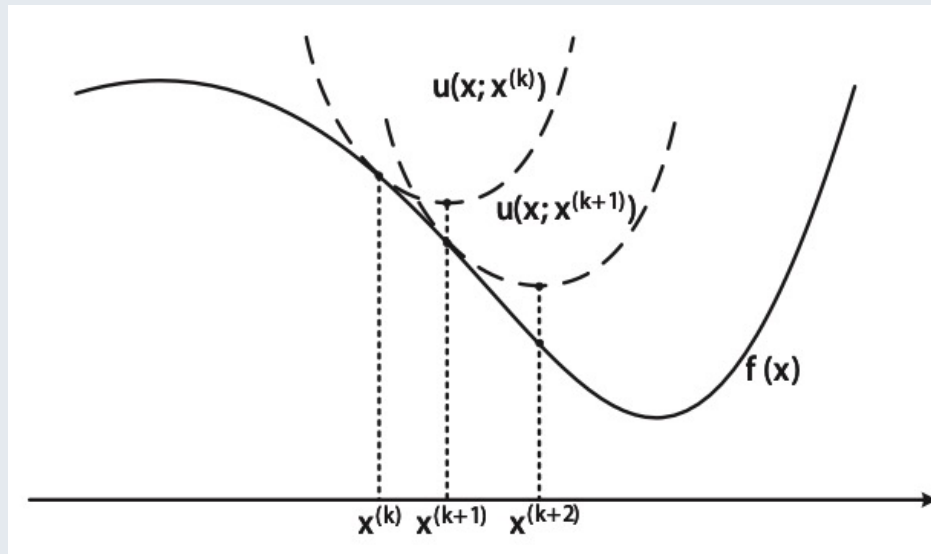
Construction rule of the surrogate / majorizer function *

$$u(\mathbf{y}, \mathbf{y}) = f(\mathbf{y}), \forall \mathbf{y} \in \mathcal{X}$$

$$u(\mathbf{x}, \mathbf{y}) \geq f(\mathbf{x}), \forall \mathbf{x}, \mathbf{y} \in \mathcal{X}$$

$$u'(\mathbf{x}, \mathbf{y}; \mathbf{d})|_{\mathbf{x}=\mathbf{y}} = f'(\mathbf{y}; \mathbf{d}), \forall \mathbf{d} \text{ with } \mathbf{y} + \mathbf{d} \in \mathcal{X}$$

$u(\mathbf{x}, \mathbf{y})$ is continuous in \mathbf{x} and \mathbf{y}



Question: how to construct $u(\mathbf{x}, \mathbf{x}^k)$?

Answer: that's more like an art :)

Luckily, the MM algorithm for l_1 -norm minimization
has been well established!

Majorizer for l_1 -norm

- Consider the following quadratic majorizer of $f(t) = |t|$ for $t \neq 0$ (for simplicity we ignore this case)

$$u(t, t^k) = \frac{1}{2|t^k|} \left(t^2 + (t^k)^2 \right).$$

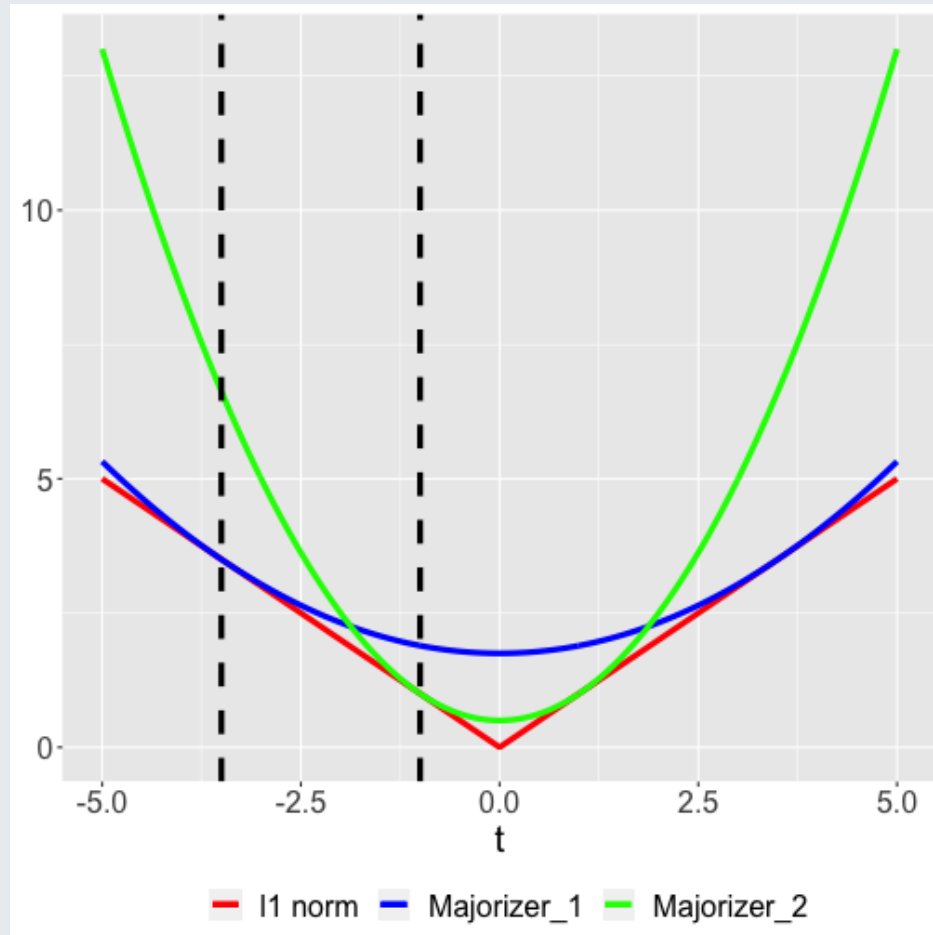
- It is a valid majorizer since it is continuous, and

$$u(t, t^k) \geq f(t),$$

$$u(t^k, t^k) = f(t^k),$$

$$\frac{d}{dt} u(t^k, t^k) = \frac{d}{dt} f(t^k).$$

Majorizer for l_1 -norm



Reweighted LS for ℓ_1 -norm minimization

- Now we can apply it to the ℓ_1 -norm: a quadratic majorizer of $f(\beta) = \|X\beta - y\|_1$ is

$$u(\beta, \beta^k) = \sum_{i=1}^N \frac{1}{2 |[X\beta^k - y]_i|} \left([X\beta - y]_i^2 + \left([X\beta^k - y]_i \right)^2 \right)$$

- Now that we have the majorizer, we can write the MM iterative algorithm for $k = 0, 1, \dots$ as

$$\underset{\beta}{\text{minimize}} \quad \|(X\beta - y) \odot w^k\|_2^2$$

where $w_i^k = \sqrt{\frac{1}{2|[X\beta^k - y]_i|}}$.

Algorithm

- Set $k = 0$ and initialize with a feasible point β^0
- **repeat**
 - $w_i^k \leftarrow \sqrt{\frac{1}{2|[X\beta^k - y]_i|}}$
 - Update $\beta^{k+1} \leftarrow \underset{\beta}{\operatorname{argmin}} \|(X\beta - y) \odot w^k\|_2^2$
 - $k \leftarrow k + 1$
- **until** convergence
- **return** β^k

Implementation (first 4 steps)


Initialize

Call `lm()`

Call `geom_smooth()`

`ggplot`

```
df <- data.frame(y = y_obs_ol, x = x_ol, weight = rep(0, length(x_ol)))  
  
#beta_0 <- rnorm(1) # Initialize intercept  
#beta_1 <- rnorm(1) # Initialize slope  
beta_0 <- -3 # To demonstrate, we fit beta_0 = -3  
beta_1 <- 1 # To demonstrate, we fit beta_1 = 1
```



Implementation (first 4 steps)

Initialize

Call lm()

Call geom_smooth()

ggplot

```
opar <- par()
par(mfrow = c(2, 2))

for (k in 0:3) { # Here we only repeat 4 times
  fit_l1 <- lm(y ~ x, data = df, weights = sqrt(1 / 2 / abs(beta_0 + x)))

  beta_0 <- coef(fit_l1)[1] # Update intercept
  beta_1 <- coef(fit_l1)[2] # Update slope

  # Visualize
  plot(x_ol, y_obs_ol, pch = 16,
       xlab = "x", ylab = "y",
       cex = 1.5, cex.axis = 1.5, cex.lab = 1.5)
  abline(fit_l1, col = "blue", lwd = 3,
        cex = 1.5, cex.axis = 1.5, cex.lab = 1.5)
}
```

Implementation (first 4 steps)

Initialize

Call lm()

Call geom_smooth()

ggplot

```
p_list <- list() # Figure list
for (k in c(1:4)) { # Here we only repeat 4 times
  df$weight <- sqrt(1 / 2 / abs(beta_0 + x_ol * beta_1 - y_obs_ol))
  fit_l1 <- lm(y ~ x, data = df, weights = weight) # Reweighted LS for
  beta_0 <- coef(fit_l1)[1] # Update intercept
  beta_1 <- coef(fit_l1)[2] # Update slope
  p <- ggplot(df, aes(x = x, y = y, size = weight / 3)) +
    geom_point(shape = 16) +
    geom_smooth(method = "lm", aes(weight = weight), size = 1.5, show.legend = FALSE)
  theme(
    text = element_text(size = 18),
    legend.title = element_text(size = 12),
    legend.text = element_text(size = 11),
    legend.position = "bottom"
  )
  p_list <- c(p_list, list(p))
}
```

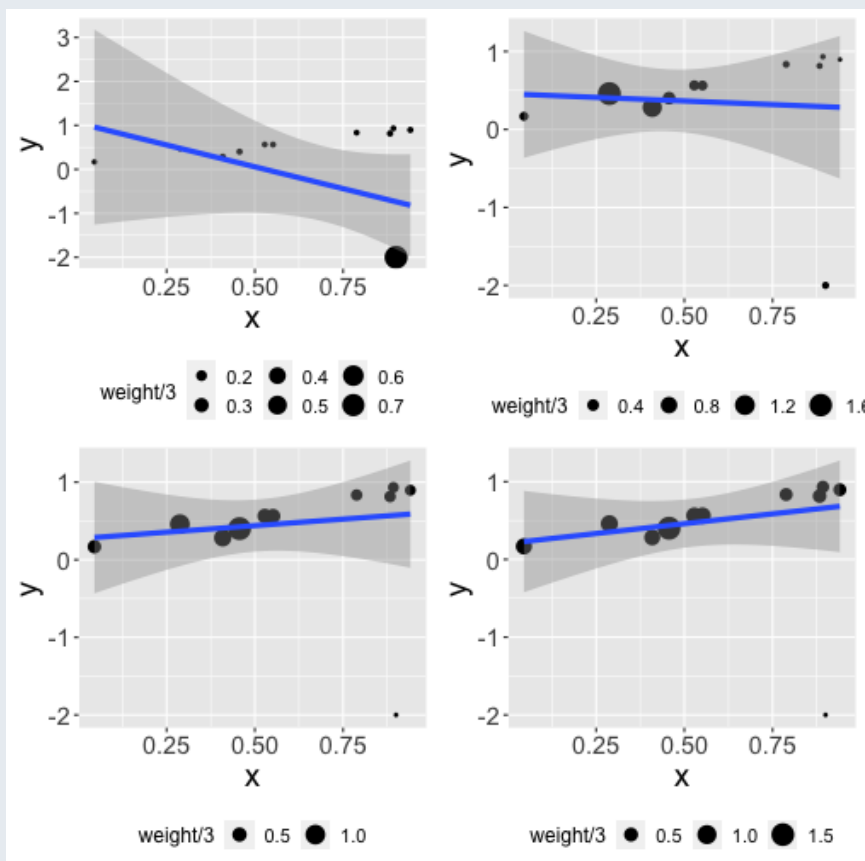
Implementation (first 4 steps)

Initialize

Call `lm()`

Call `geom_smooth()`

ggplot



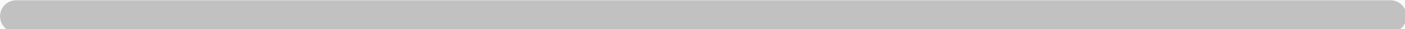
Full implementation

Initialize

ℓ_1 norm minimization

Visualization

```
df <- data.frame(y = y_obs_ol, x = x_ol, weight = rep(0, length(x_ol)))  
  
#beta_0 <- rnorm(1) # Initialize intercept  
#beta_1 <- rnorm(1) # Initialize slope  
beta_0 <- -3 # To demonstrate, we fit beta_0 = -3  
beta_1 <- 1 # To demonstrate, we fit beta_1 = 1  
  
tol <- 1e-6 # Convergence tolerance / criterion  
iter_max <- 5000 # Maximum number of iterations
```



Full implementation

Initialize

l1 norm minimization

Visualization

```
l1_loss <- sum(abs(beta_0 + x_ol * beta_1 - y_obs_ol)) # l1 loss at ini
for (k in 1:iter_max) {
  df$weight <- sqrt(1 / 2 / abs(beta_0 + x_ol * beta_1 - y_obs_ol))
  fit_l1 <- lm(y ~ x, data = df, weights = weight) # Reweighted LS for
  beta_0 <- coef(fit_l1)[1] # Update intercept
  beta_1 <- coef(fit_l1)[2] # Update slope

  l1_loss_current <- sum(abs(beta_0 + x_ol * beta_1 - y_obs_ol)) # l1 l
  l1_loss <- c(l1_loss, l1_loss_current)

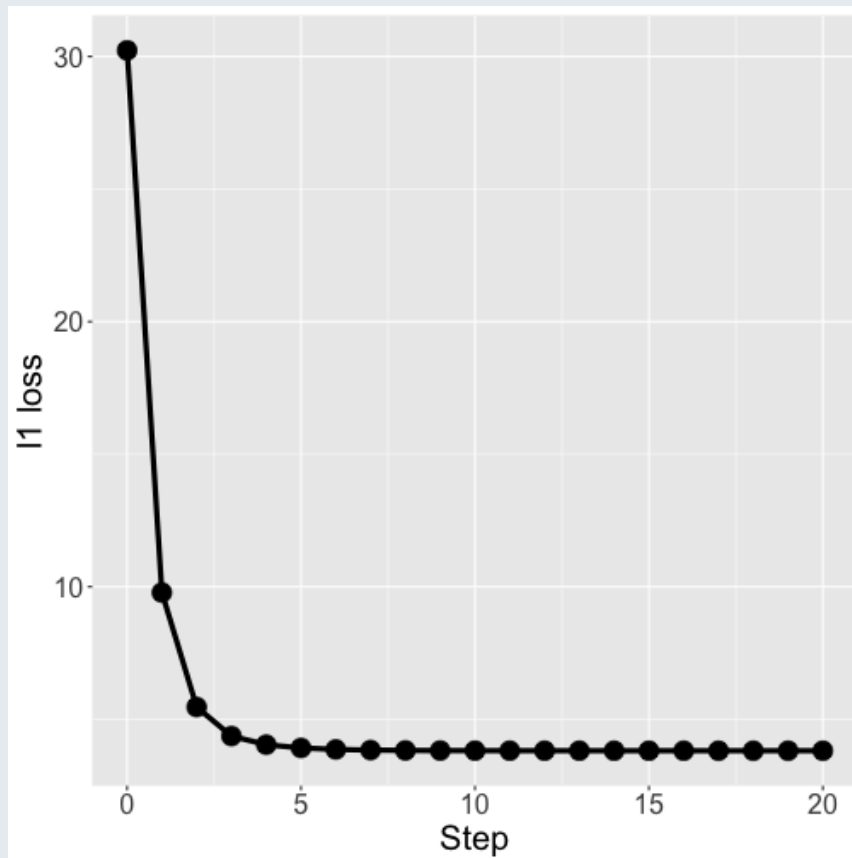
  # Whether converges
  if(abs((l1_loss[k + 1] - l1_loss[k]) / l1_loss[k]) < tol){
    break
  }
}
```

Full implementation

Initialize

ℓ_1 norm minimization

Visualization



Good night!

Slides created via Yihui Xie's R package [xaringan](#).

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The chakra comes from [remark.js](#), [knitr](#), and [R Markdown](#).