T04: Outliers and l_1 loss

MATH 4432 Statistical Machine Learning

WANG Zhiwei

MATH, HKUST

2022-09-27

Let's start by recalling linear regression!

Least squares

Recall the least squares (LS) problem for linear regression

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

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

Least squares

Recall the least squares (LS) problem for linear regression

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

A toy example | Code | Minimize the squared loss

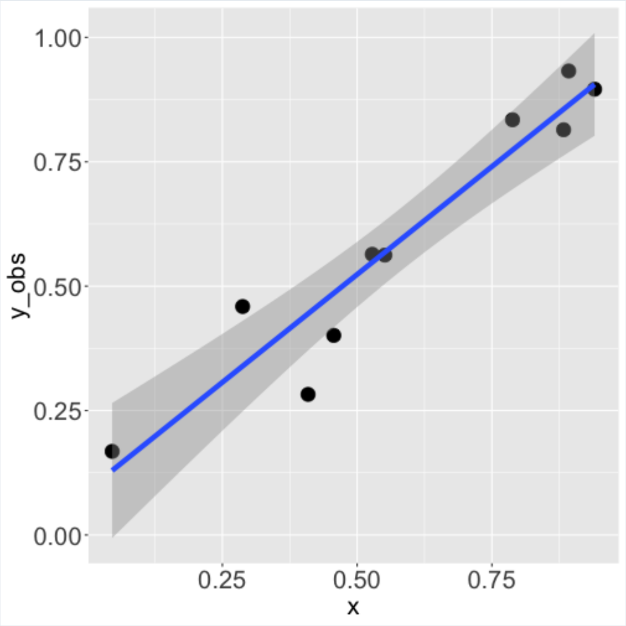
```
set.seed(123)
N <- 10 # Sample size
x <- runif(N, 0, 1)
y0 <- x # Ground truth
y_obs <- y0 + rnorm(N, mean = 0, sd = 0.1) # Add noise, observed data
ggplot(data = NULL, aes(x = x, y = y_obs)) +
  geom_point(aes(x = x, y = y_obs), size = 5) +
  geom_smooth(method = "lm", size = 2) +
  theme(
    text = element_text(size = 20),
    axis.text.y = element_text(size = 20),
    axis.text.x = element_text(size = 20)
    )
```

Least squares

Recall the least squares (LS) problem for linear regression

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

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

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

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

Add an outlier

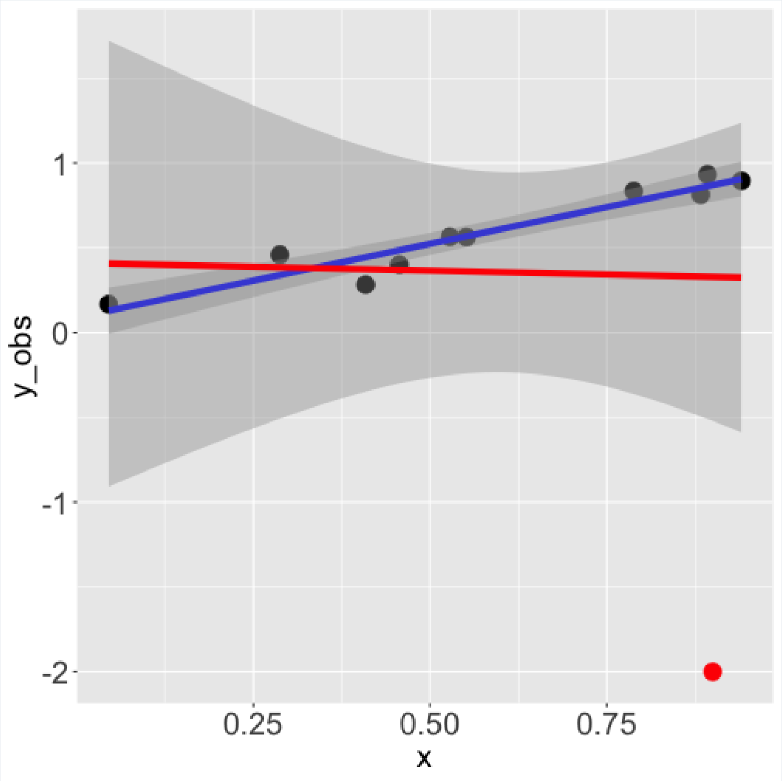
Add an outlier | **Code** | Minimize the squared loss

```
x_ol <- c(x, 0.9)
y0_ol <- c(y0, 0.9)
y_obs_ol <- c(y_obs, -2)

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
  geom_smooth(aes(x = x_ol, y = y_obs_ol), method = "lm", color = "red",
  theme(
    text = element_text(size = 20),
    axis.text.y = element_text(size = 20),
    axis.text.x = element_text(size = 20)
    )
```

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

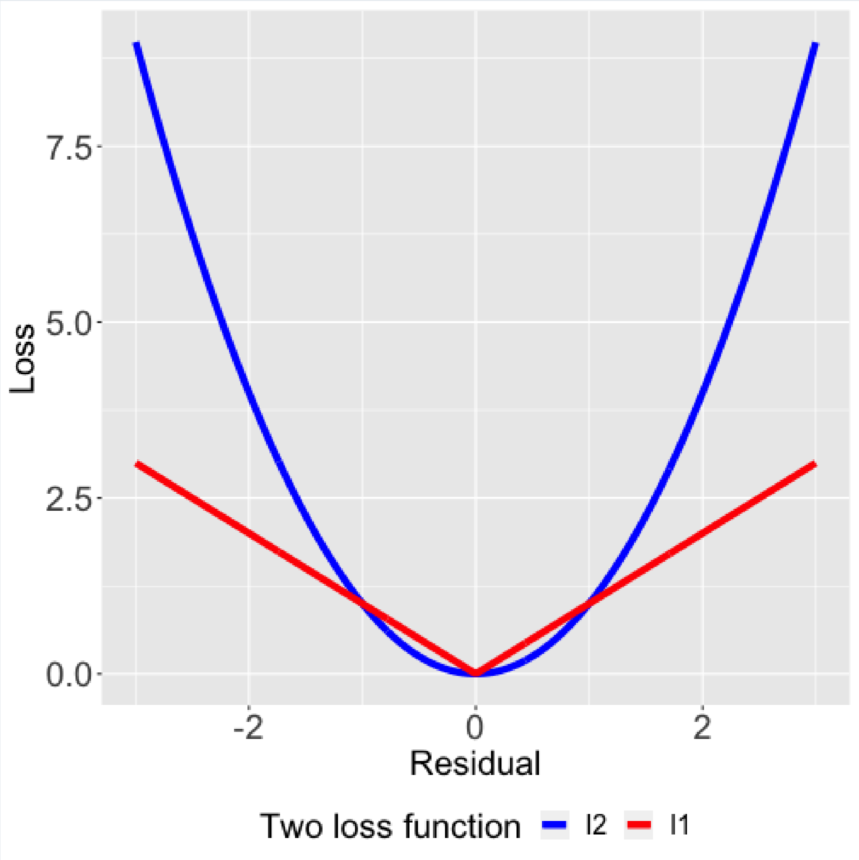
$$||x||_2 = \left(\sum_{j=1}^{p} x_j^2\right)^{\frac{1}{2}}, \quad ||x||_1 = \sum_{j=1}^{p} |x_j|.$$

- l_2 loss and l_1 loss

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

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

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 managable surrogate function $u\left(\mathbf{x}, \mathbf{x}^k\right)$

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

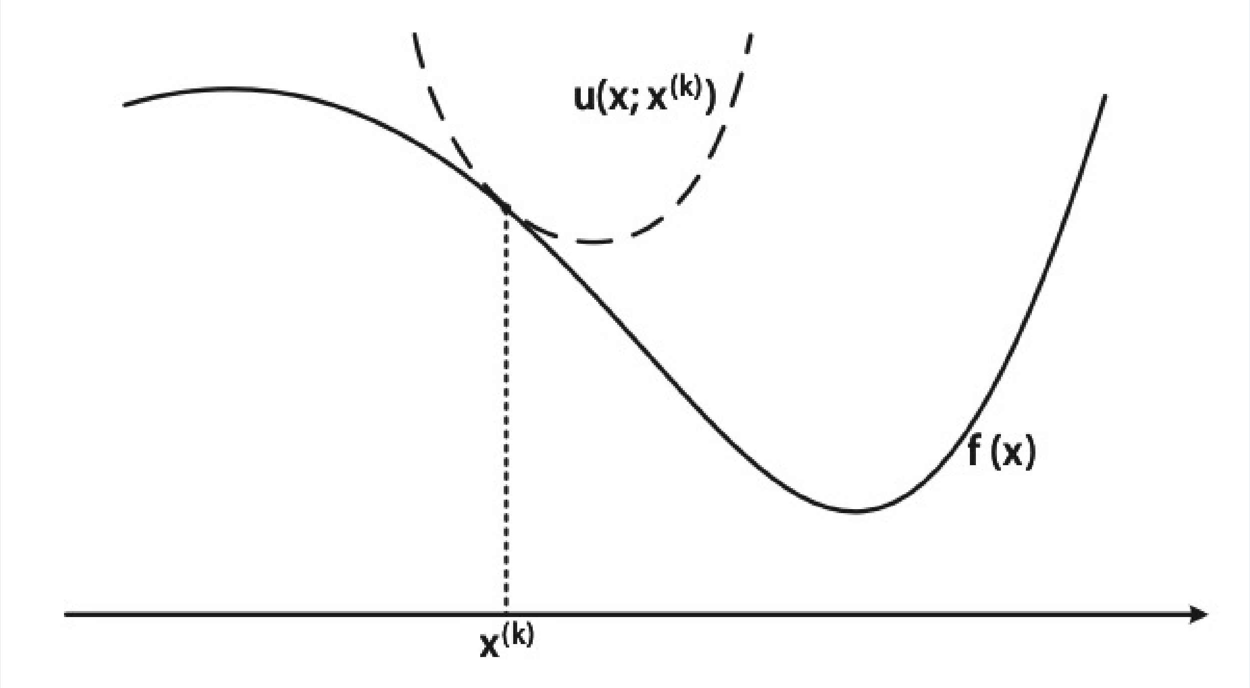
  hoping the sequence of minimizers $\left\{\mathbf{x}^k\right\}$ will converge to optimal $\mathbf{x}^\star$.

[*] Not required in this course. Materials are form 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 $x_{k-1} \to x_k$.

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 $x_{k-1} \to x_k$.

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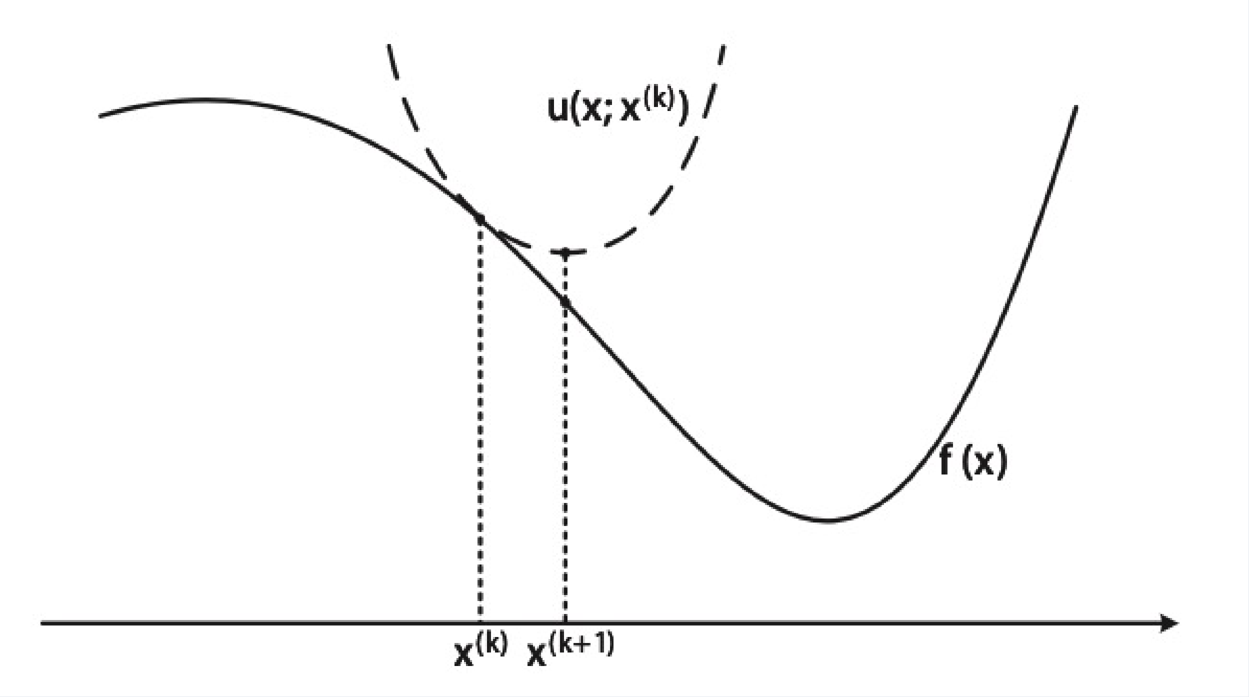
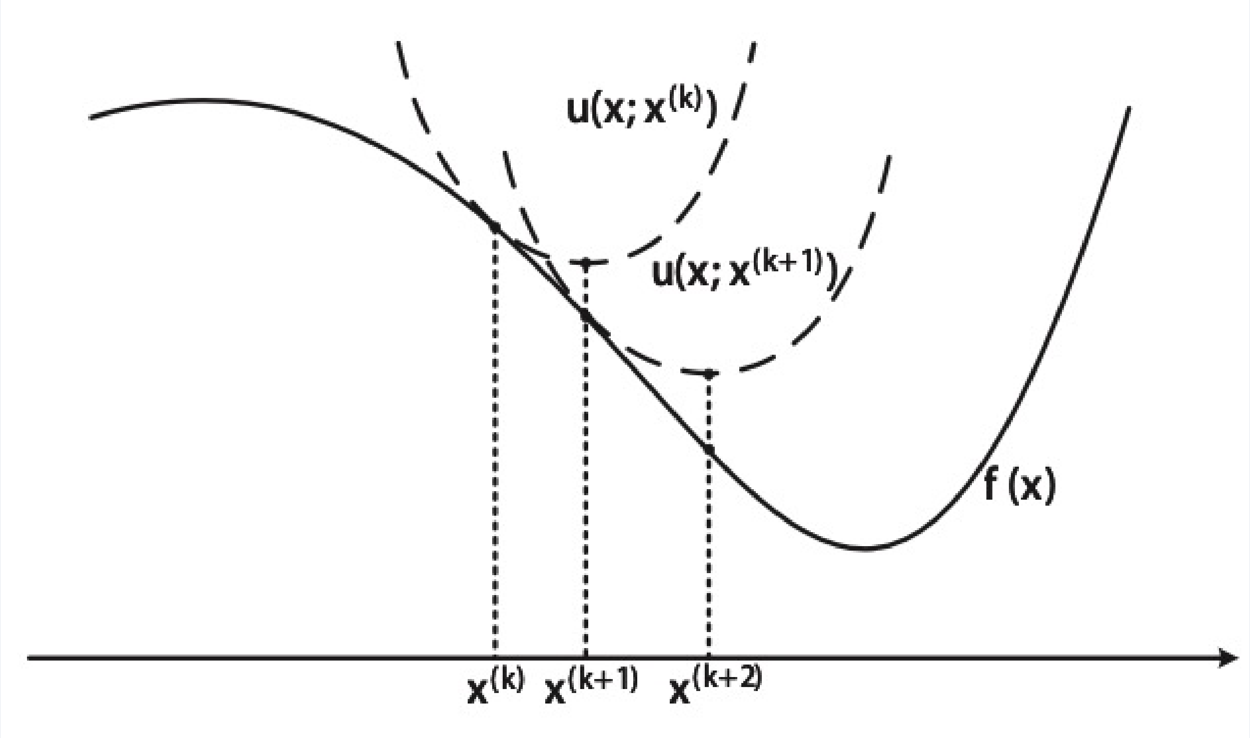


Iterative algorithm

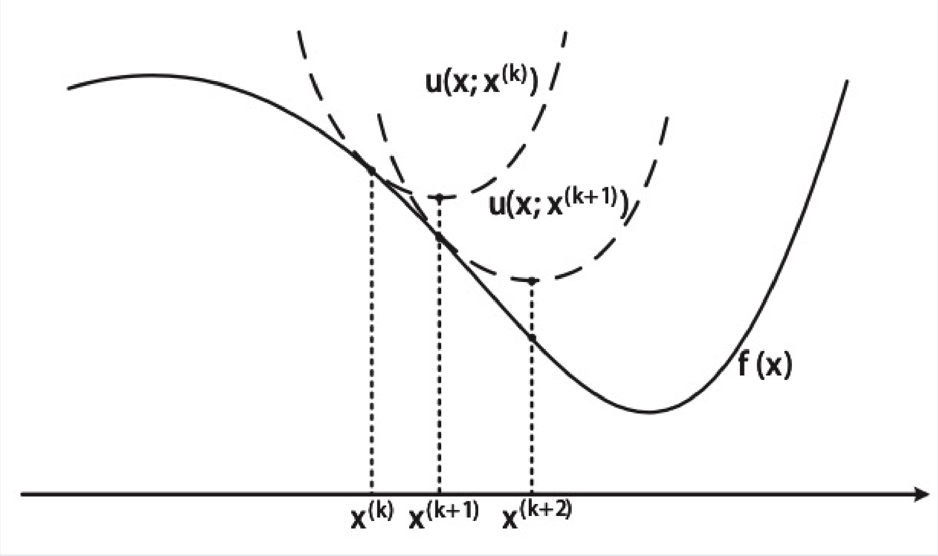
Suppose x_0 is the initial point, in k-th step, we want $x_{k-1} \to x_k$.

After k-th step (k+1)-th step **(k+2)-th step**



Construction rule of the surrogate / majorizer function *

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



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

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)

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

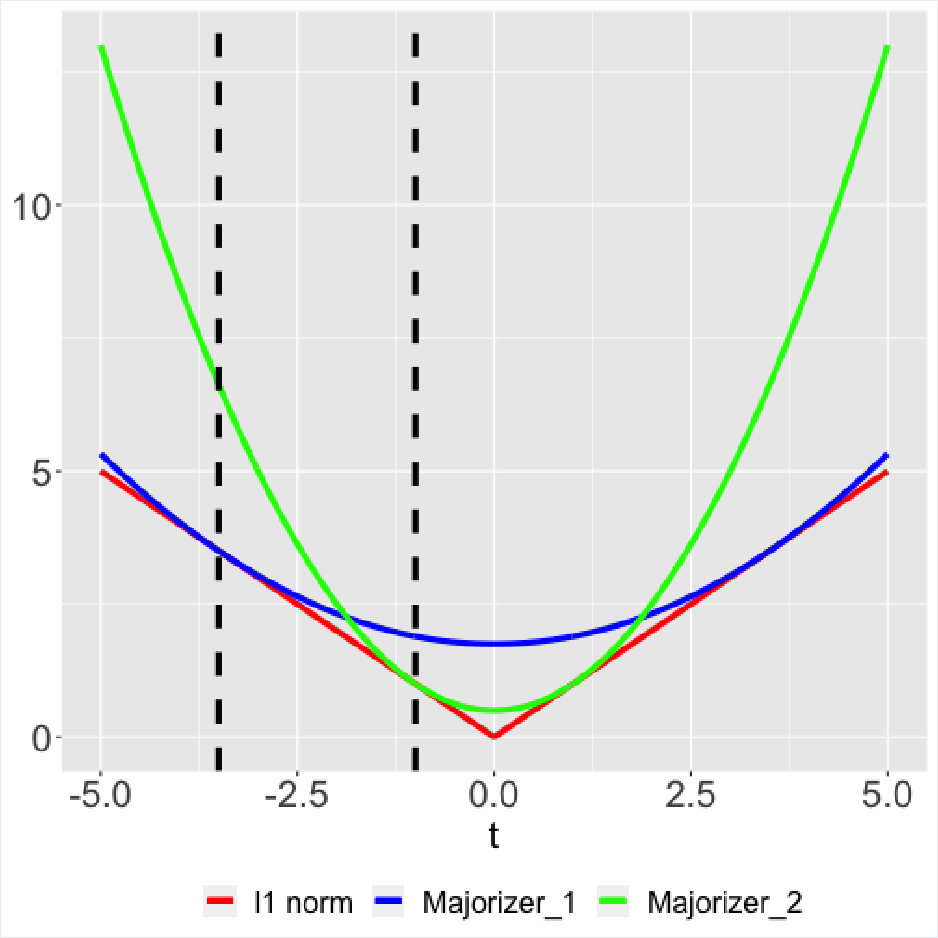
- It is a valid majorizer since it is continuous, and

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

$$u\left(t^k, t^k\right) = f(t),$$

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

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

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

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

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

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

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 $\beta^{k+1} \leftarrow \underset{\beta}{\operatorname{argmin}} \left\|(X\beta - y) \odot w^k\right\|_2^2$
  - $k \leftarrow k + 1$
- **until** convergence
- **return** β^k

Implementation (first 4 steps)

Initialization | lm() | 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)

Initialization | lm() | 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)
}
```

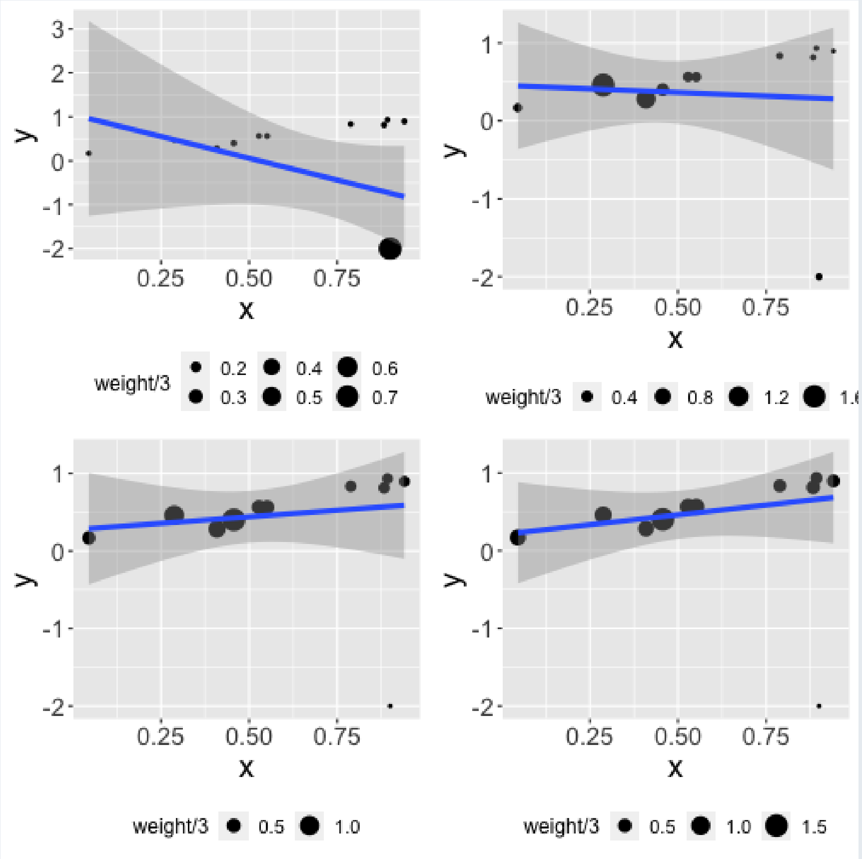
Implementation (first 4 steps)

Initialization | lm() | **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.le
    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)

Initialization | lm() | geom_smooth() | ggplot



Full implementation

Initialization and parameter setting | l1 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
```

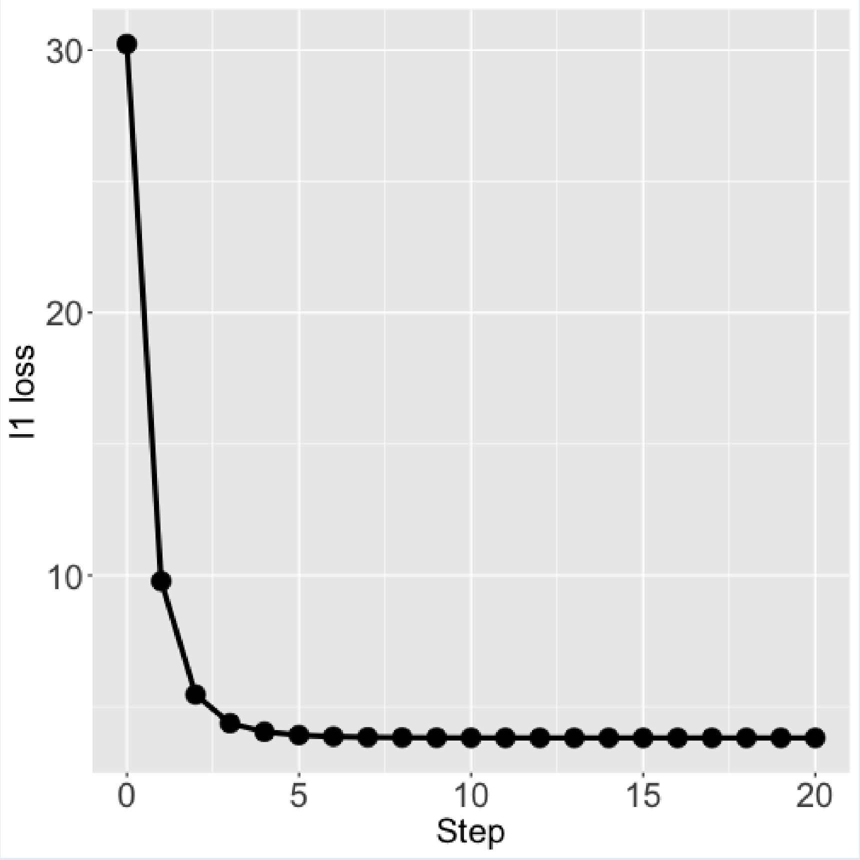
Full implementation

Initialization and parameter setting | 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 lo
  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

Initialization and parameter setting | l1 norm minimization | **Visualization**



Subgradient method *

We say a vector $g \in \mathbf{R}^n$ is a subgradient of $f : \mathbf{R}^n \to \mathbf{R}$ at $x \in \mathrm{dom}\, f$ if for all $z \in \mathrm{dom}\, f$,

$$f(z) \geq f(x) + g^T(z - x).$$

The subgradient of l_1-norm can be taken as

$$g_i = \begin{cases} +1 & x_i > 0 \\ -1 & x_i < 0 \\ [-1, \ +1] & x_i = 0 \end{cases}.$$

Note: subgradient method is **not** a descent method, and negative subgradient is **not** always a descent direction!

[*] Materials are from Subgradients and Subgradient Methods, Stephen Boyd and Lieven Vandenberghe, EE364b, Stanford University.

Implementation

Initialization and parameter setting | Implementation | Visualization

```
X <- cbind(x0 = rep(1, length(x_ol)), x1 = x_ol)
beta <- c(beta_0 = -3, beta_1 = 1) # Initialize
l1_loss <- sum(abs(beta[1] + x_ol * beta[2] - y_obs_ol)) # l1 loss at i

step_size <- 0.05 # Try different step size, e.g., 0.1 and 0.01, and se
tol <- 1e-3 # Convergence tolerance / criterion
iter_max <- 5000 # Maximum number of iterations
```

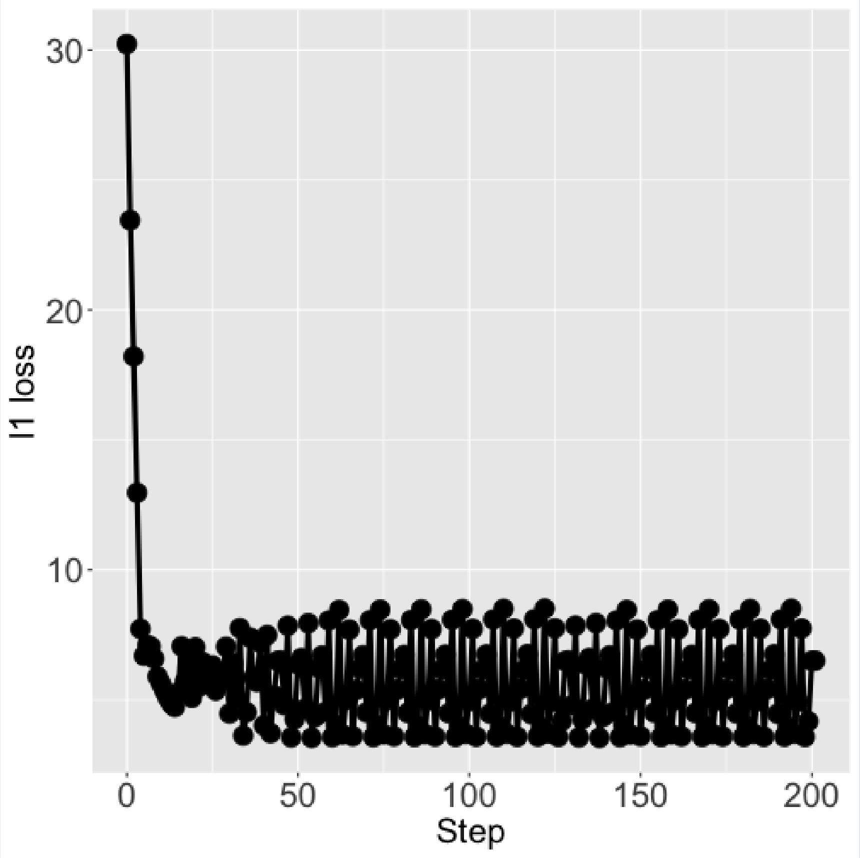
Implementation

Initialization and parameter setting | **Implementation** | Visualization

```
for (k in 1:iter_max) {
  r <- as.vector(y_obs_ol - X %*% as.matrix(c(beta))) # Residual
  subgrad <- colSums(X * sign(r)) # Subgradients

  beta <- beta + step_size * subgrad # Update beta

  l1_loss_current <- sum(abs(beta[1] + x_ol * beta[2] - y_obs_ol)) # l1
  l1_loss <- c(l1_loss, l1_loss_current)

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

Implementation

Initialization and parameter setting | Implementation | **Visualization**



Good night!

Slides created via Yihui Xie's R package **xaringan**.

Theme customized via Garrick Aden-Buie's R package **xaringanthemer**.

Tabbed panels created via Garrick Aden-Buie's R package **xaringanExtra**.

The chakra comes from remark.js, **knitr**, and R Markdown.