TO4: 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

$$\hat{eta} = rgmin_{eta} \sum_{i=1}^N (y_i - x_i eta)^2 = rgmin_{eta} rac{1}{N} \sum_{i=1}^N (y_i - x_i eta)^2.$$

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

Least squares

Recall the least squares (LS) problem for linear regression

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A tov example

Code Minimize the squared loss

```
set.seed(123)
N <- 10 # Sample size
x \leftarrow 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

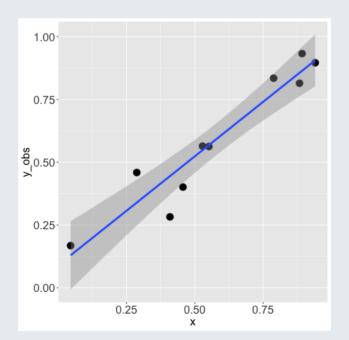
Recall the least squares (LS) problem for linear regression

$$\hat{eta} = rgmin_{eta} \sum_{i=1}^N (y_i - x_i eta)^2 = rgmin_{eta} rac{1}{N} \sum_{i=1}^N (y_i - x_i eta)^2.$$

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

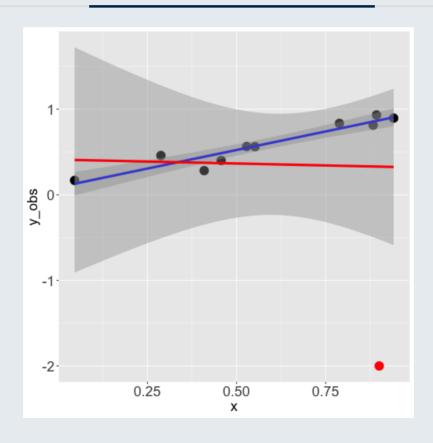
```
set.seed(123)
x ol < -c(x, 0.9)
v0 \text{ ol} <- c(v0, 0.9)
y_obs_ol <- c(y_obs, -2) # Add noise, observed data
ggplot(data = NULL) +
  geom_point(aes(x = x, y = y_obs), size = 5) +
  geom_point(aes(x = 0.9, y = -2), color = "red", size = 5) +
  geom_smooth(aes(x = x, y = y_obs), method = "lm", color = "blue", size
  geom\_smooth(aes(x = x_ol, y = y_obs_ol), method = "lm", color = "red")
  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!

l₁ loss

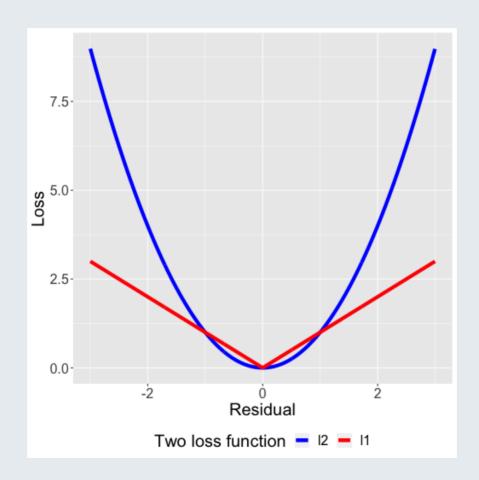
• l_2 norm and l_1 norm

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

• l_2 loss and l_1 loss

$$egin{aligned} \mathcal{L}_2 &= \sum_{i=1}^N (y_i - x_i eta)^2 = ||y - X eta||_2^2, \ \mathcal{L}_1 &= \sum_{i=1}^N |y_i - x_i eta| = ||y - X eta||_1. \end{aligned}$$

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

$$\text{minimize } f(\mathbf{x})$$
 $\text{subject to } \mathbf{x} \in \mathcal{X},$

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

ullet Idea: successively minimize a more managable surrogate function $u\left(\mathbf{x},\mathbf{x}^k
ight)$

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

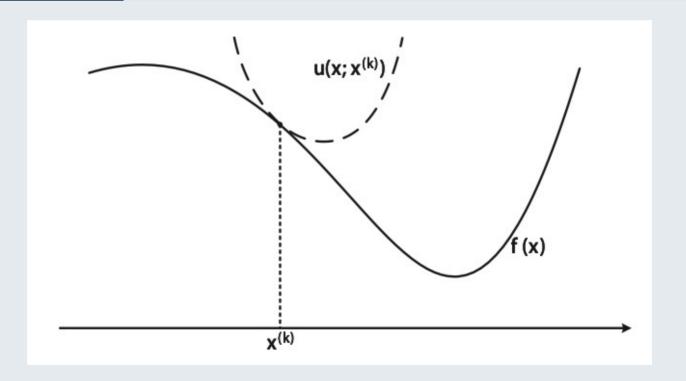
hoping the sequence of minimizers $\left\{\mathbf{x}^k\right\}$ will converge to optimal \mathbf{x}^\star .

[*] 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 $x_{k-1} \to x_k$.

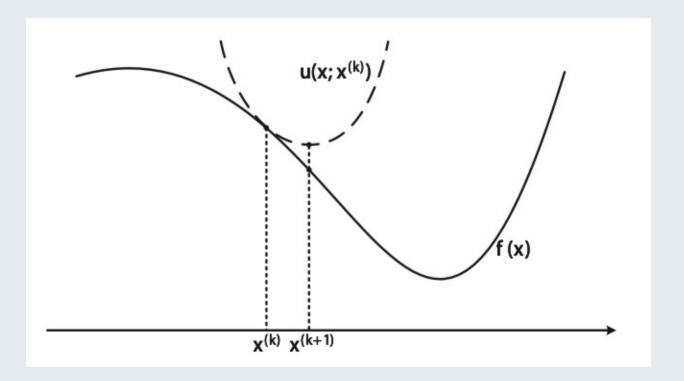
After k-th step (k+1)-th step (k+2)-th step



Iterative algorithm

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

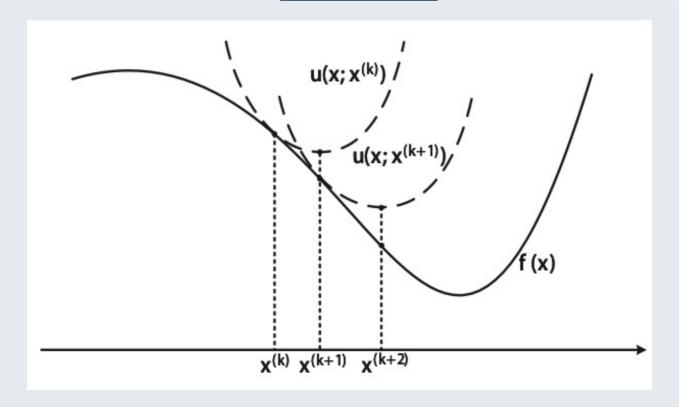
After k-th step (k+1)-th step (k+2)-th step



Iterative algorithm

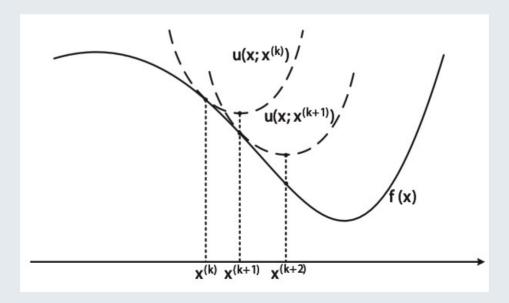
Suppose x_0 is the initial point, in k-th step, we want $x_{k-1} \to x_k$.

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



Construction rule of the surrogate / majorizer function *

$$egin{aligned} u(\mathbf{y},\mathbf{y}) &= f(\mathbf{y}), orall \mathbf{y} \in \mathcal{X} \ u(\mathbf{x},\mathbf{y}) &\geq f(\mathbf{x}), orall \mathbf{x}, \mathbf{y} \in \mathcal{X} \ u'(\mathbf{x},\mathbf{y};\mathbf{d})|_{\mathbf{x}=\mathbf{y}} &= f'(\mathbf{y};\mathbf{d}), orall \mathbf{d} ext{ with } \mathbf{y} + \mathbf{d} \in \mathcal{X} \ u(\mathbf{x},\mathbf{y}) ext{ is continuous in } \mathbf{x} ext{ and } \mathbf{y} \end{aligned}$$



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

Answer: that's more like an art:)

Luckily, the MM algorithm for l₁-norm minimization has been well established!

Majorizer for l₁-norm

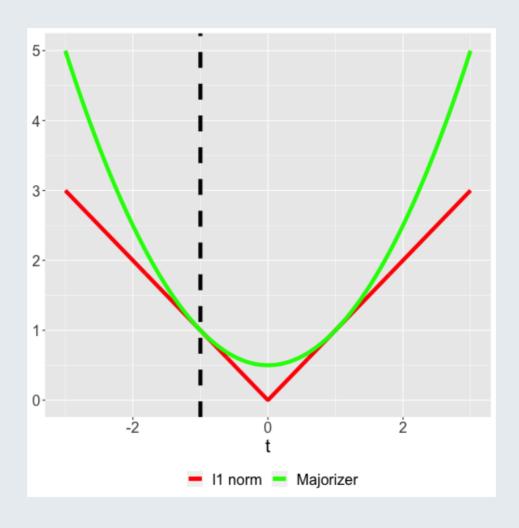
ullet Consider the following quadratic majorizer of f(t)=|t| for t
eq 0 (for simplicity we ignore this case)

$$u\left(t,t^{k}
ight)=rac{1}{2\leftert t^{k}
ightert}\Bigl(t^{2}+\left(t^{k}
ight)^{2}\Bigr)\,.$$

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

$$egin{aligned} u\left(t,t^k
ight)&\geq f(t),\ u\left(t^k,t^k
ight)&=f(t),\ rac{d}{dt}u\left(t^k,t^k
ight)&=rac{d}{dt}f\left(t^k
ight). \end{aligned}$$

Majorizer for l₁-norm



Reweighted LS for 11-norm minimization

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

$$u\left(eta,eta^k
ight) = \sum_{i=1}^N rac{1}{2\left|\left[Xeta^k-y
ight]_i
ight|}igg([Xeta-y]_i^2 + \left(\left[Xeta^k-y
ight]_iigg)^2igg)$$

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

$$\min_{eta} \left| \left(Xeta - y
ight) \odot w^k
ight|_2^2$$

where
$$w_i^k = \sqrt{rac{1}{2|[Xeta^k - y]_i|}}.$$

Algorithm

- Set k=0 and initialize with a feasible point eta^0
- repeat

$$\circ \ w_i^k \leftarrow \sqrt{rac{1}{2|[Xeta^k-y]_i|}}$$

$$\circ \hspace{0.1cm} \mathsf{Update} \hspace{0.1cm} eta^{k+1} \leftarrow \operatorname*{argmin} ig\| (Xeta - y) \odot w^k ig\|_2^2$$

$$\circ$$
 $k \leftarrow k+1$

- until convergence
- return β^k

```
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 demostrate, we fit beta_0 = -3
beta_1 <- 1 # To demostrate, we fit beta_1 = 1</pre>
```

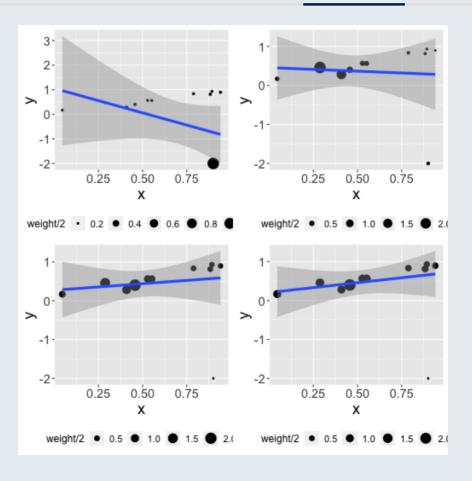
Initialize Call Im() Call geom_smooth() ggplot

```
opar <- par()
par(mfrow = c(2, 2))
for (k in 0:3) { # Here we only repeat 4 times
  fit_l1 <- lm(y \sim x, data = df, weights = sqrt(1 / 2 / abs(beta_0 + x))
  beta_0 <- coef(fit_l1)[1] # Update intercept</pre>
  beta_1 <- coef(fit_l1)[2] # Update slope</pre>
  # 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)
}
```

Initialize Call lm() Call geom smooth() ggplot

```
p list <- list() # Figure list</pre>
for (k in c(0:3)) { # 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</pre>
  beta_1 <- coef(fit_l1)[2] # Update slope</pre>
  p \leftarrow ggplot(df, aes(x = x, y = y, size = weight / 2)) +
    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))</pre>
```

Initialize Call Im() Call geom_smooth() ggplot



Good night!

Slides created via Yihui Xie's R package <u>xaringan</u>.

Theme customized via Garrick Aden-Buie's R package <u>xaringanthemer</u>.

Tabbed panels created via Garrick Aden-Buie's R package <u>xaringanExtra</u>.

The chakra comes from <u>remark.js</u>, <u>knitr</u>, and <u>R Markdown</u>.