CPSC 340: Machine Learning and Data Mining

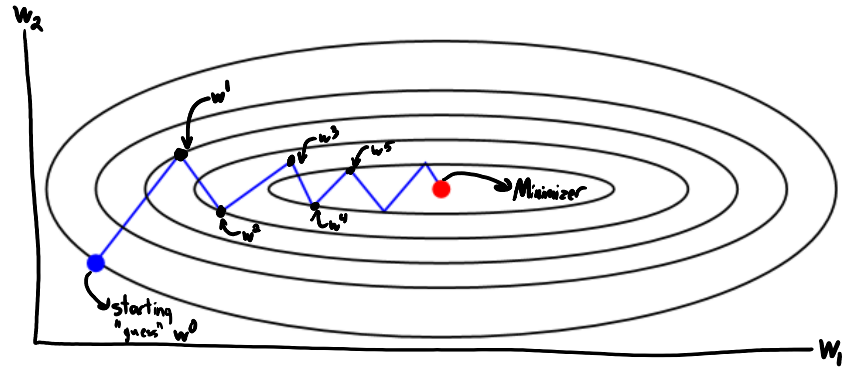
Robust Regression

Fall 2020

Last Time: Gradient Descent and Convexity

- We introduced gradient descent:
  - Uses sequence of iterations of the form:

$$w^{t+1} = w^t - \alpha^t \nabla f(w^t)$$



  - Converges to a stationary point where ∇ f(w) = 0 under weak conditions.
    - Will be a global minimum if the function is convex.
- We discussed ways to show a function is convex:
  - Second derivative is non-negative (1D functions).
  - Closed under addition, multiplication by non-negative, maximization.
  - Any [squared-]norm is convex.
  - Composition of convex function with linear function is convex.

Example: Convexity of Linear Regression

- Consider linear regression objective with squared error:

$$f(w) = \|Xw - y\|^2$$

- We can use that this is a convex function composed with linear:

Let $h(w) = Xw - y$, which is a linear function ('d' inputs, 'n' outputs)
Let $g(r) = \|r\|^2$, which is convex because it's a squared norm.
Then $f(w) = g(h(w))$, which is convex because it's a convex function composed with a linear function

Convexity in Higher Dimensions

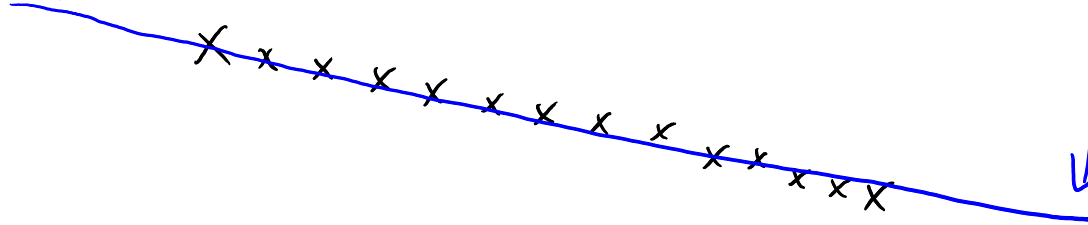
- Twice-differentiable 'd'-variable function is convex iff:
  - Eigenvalues of Hessian $\nabla^2 f(w)$ are non-negative for all 'w'.
- True for least squares where $\nabla^2 f(w)$ = X^TX for all 'w'.
  - It may not be obvious that this matrix has non-negative eigenvalues.
- Unfortunately, sometimes it is hard to show convexity this way.
  - Usually easier to just use some of the rules as we did on the last slide.

(pause)

Least Squares with Outliers

- Consider least squares problem with outliers in ‘y’:

x ← “outlier” that doesn't follow trend

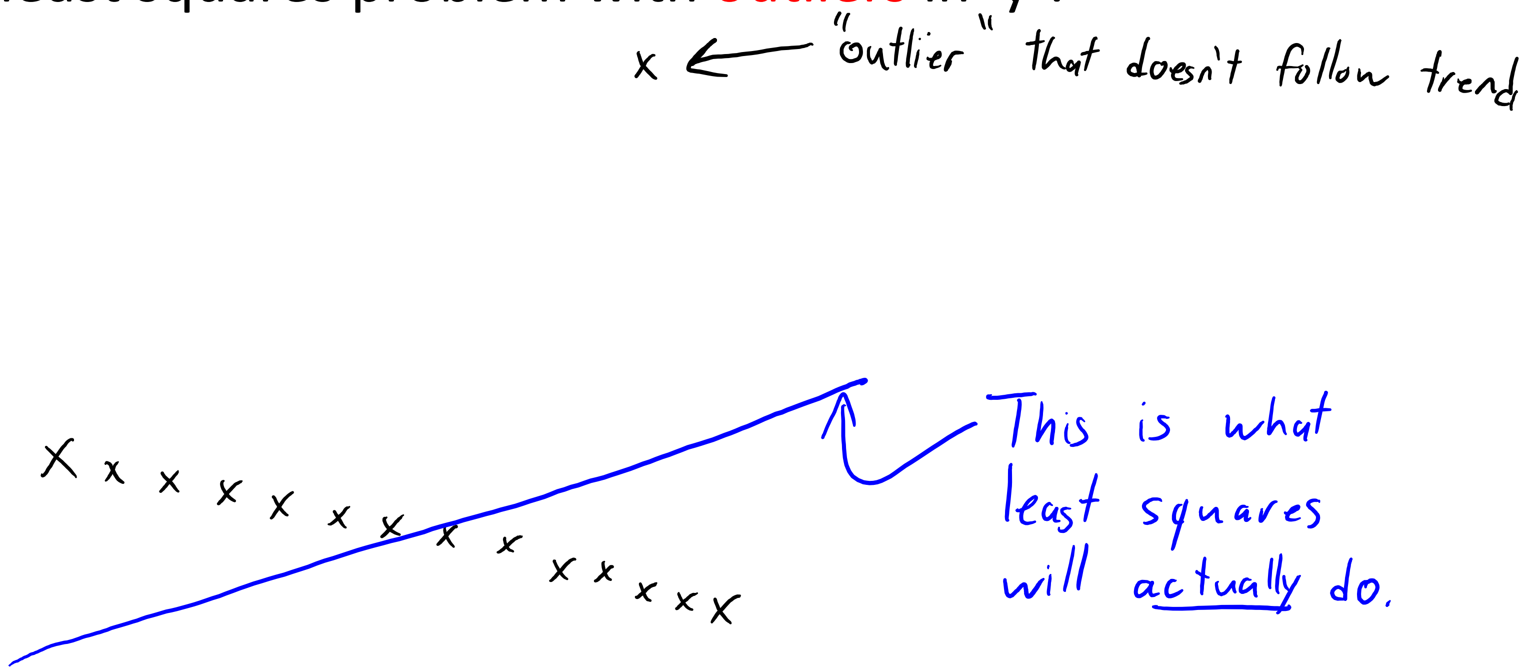


This is what we *want* least squares to do.

http://setosa.io/ev/ordinary-least-squares-regression

Least Squares with Outliers

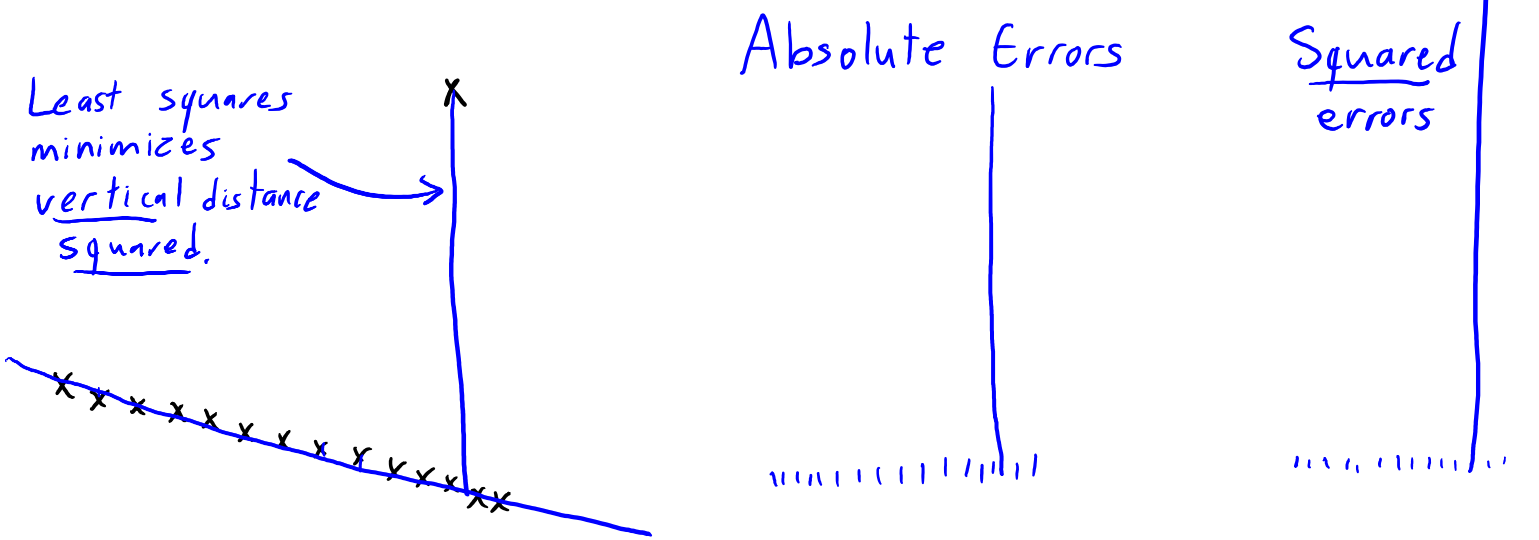
- Consider least squares problem with outliers in 'y':



- Least squares is very sensitive to outliers.

Least Squares with Outliers

- Squaring error shrinks small errors, and magnifies large errors:

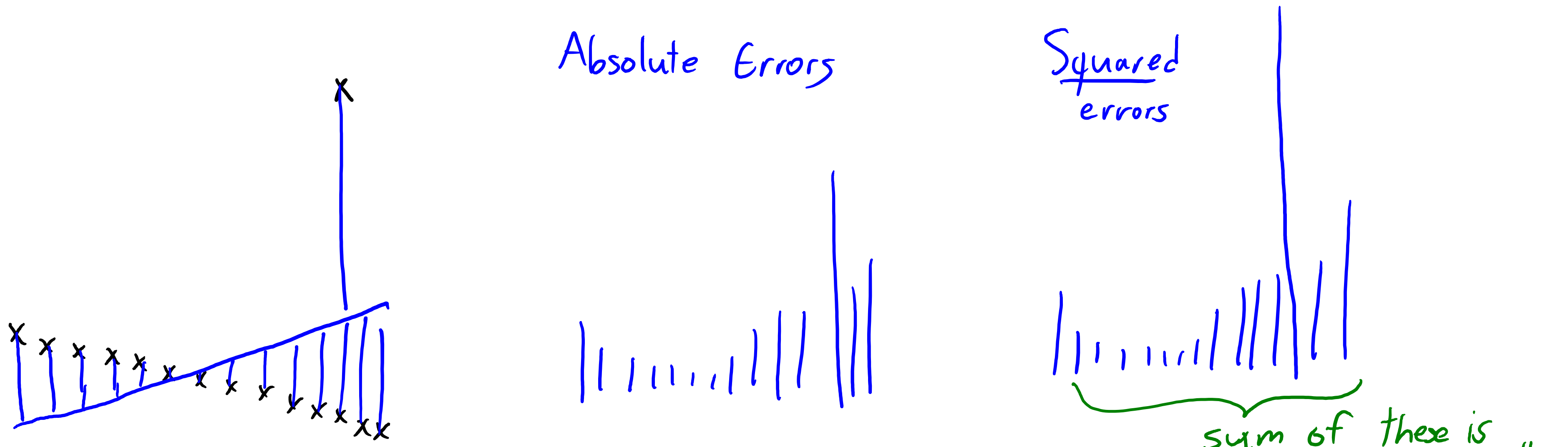


- Outliers (large error) influence ‘w’ much more than other points.

https://seeing-theory.brown.edu/regression-analysis/index.html

Least Squares with Outliers

- Squaring error shrinks small errors, and magnifies large errors:



- Outliers (large error) influence 'w' much more than other points.
  - Good if outlier means 'plane crashes', bad if it means 'data entry error'.

smaller than for the "correct" line.

Robust Regression

- Robust regression objectives focus less on large errors (outliers).
- For example, use absolute error instead of squared error:

$$f(w) = \sum_{i=1}^{n} |w^T x_i - y_i|$$

- Now decreasing 'small' and 'large' errors is equally important.
- Instead of minimizing L2-norm, minimizes L1-norm of residuals:

Least squares:

$$f(w) = \frac{1}{2}\|Xw - y\|^2$$

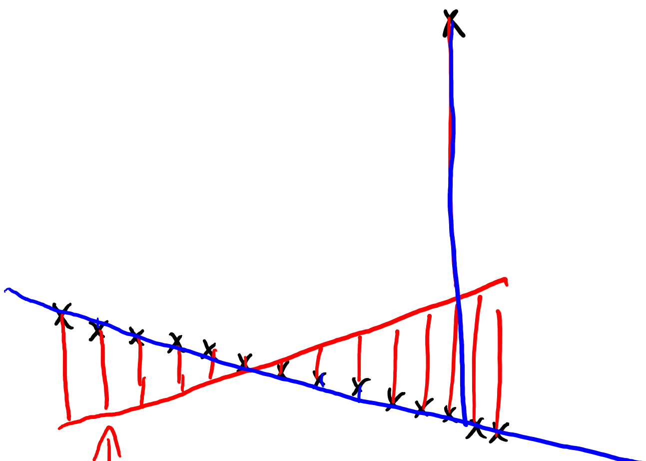
Least absolute error:

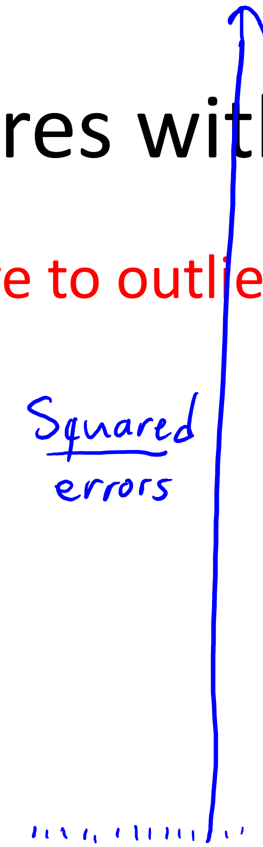
$$f(w) = \|Xw - y\|_1$$

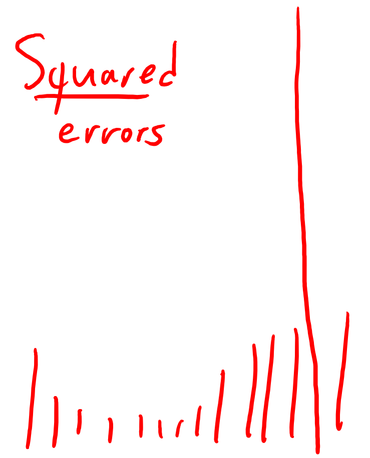
$$\sum_{i=1}^{n} |w^T x_i - y_i| = \sum_{i=1}^{n} |r_i| = \|r\|_1 = \|Xw - y\|_1$$

Least Squares with Outliers

- Least squares is very sensitive to outliers.



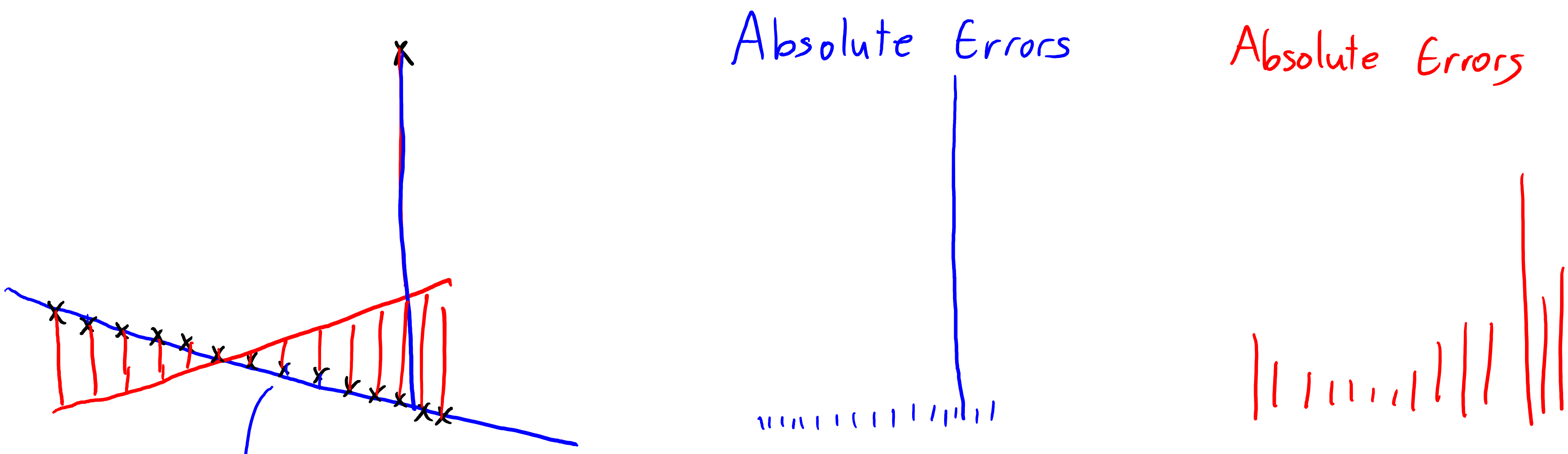




Linear model 'w' minimizing $f(w) = \frac{1}{2}\|Xw - y\|^2$

Least Squares with Outliers

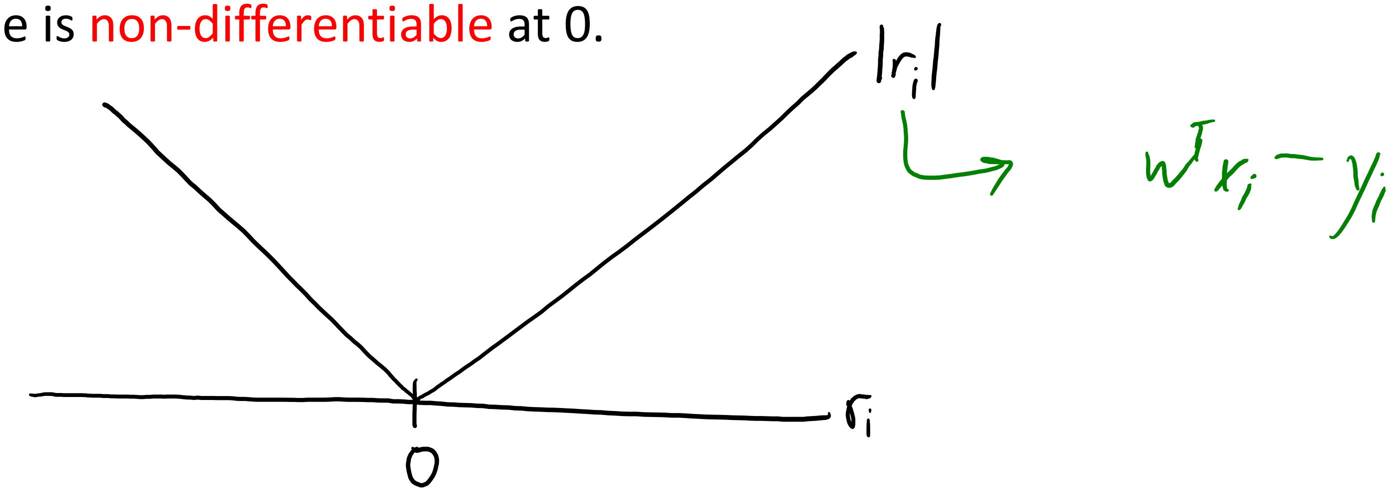
- Absolute error is more robust to outliers:



Linear model 'w' minimizing $f(w) = \|Xw - y\|_1 = \sum_{i=1}^{n} |w^T x_i - y_i|$

Regression with the L1-Norm

- Unfortunately, minimizing the absolute error is harder.
  - We don't have "normal equations" for minimizing the L1-norm.
  - Absolute value is non-differentiable at 0.



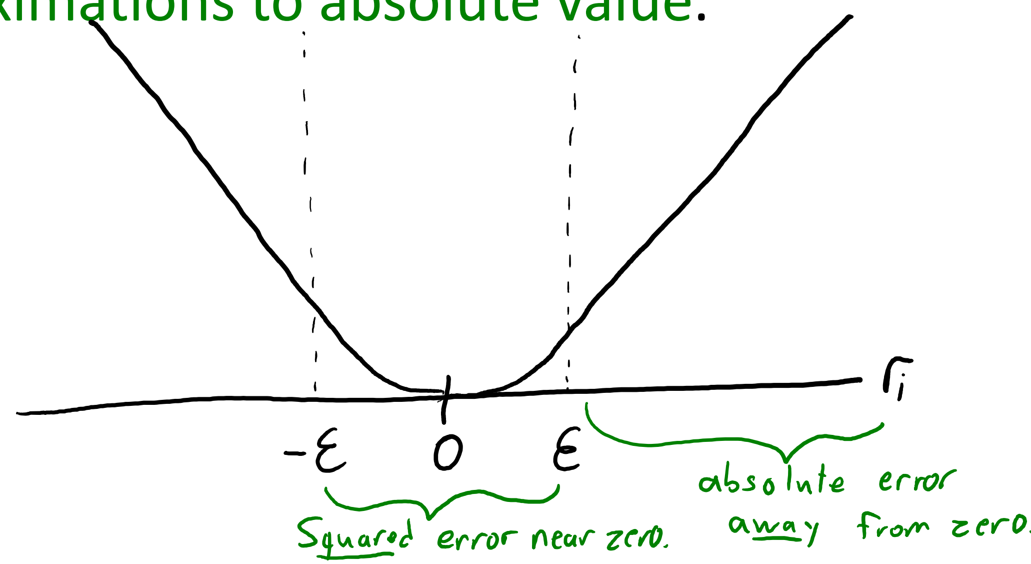
  - Generally, harder to minimize non-smooth than smooth functions.
    - Unlike smooth functions, the gradient may not get smaller near a minimizer.
  - To apply gradient descent, we'll use a smooth approximation.

Smooth Approximations to the L1-Norm

- There are differentiable approximations to absolute value.
  - Common example is Huber loss:

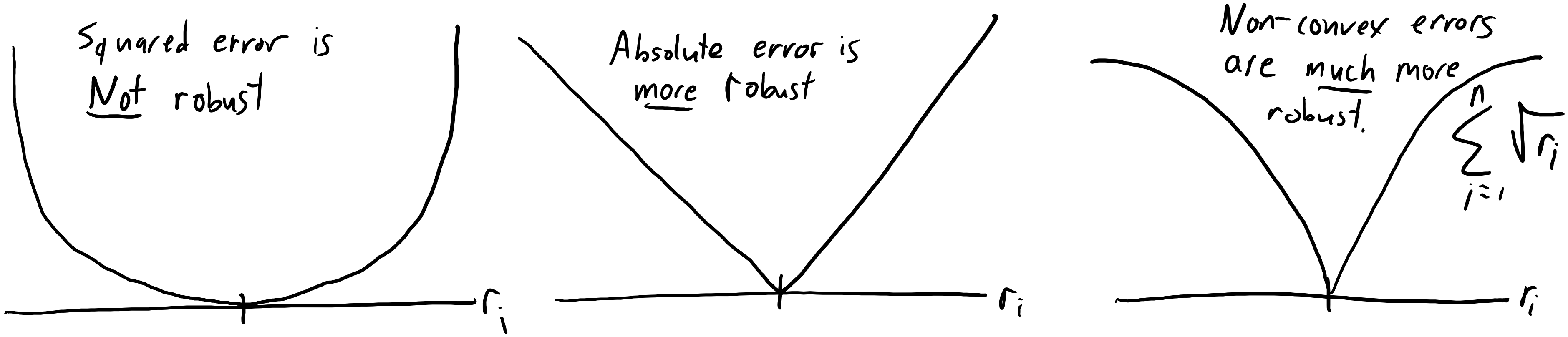
$$f(w) = \sum_{i=1}^{n} h(w^T x_i - y_i)$$

$$h(r_i) = \begin{cases} \frac{1}{2} r_i^2 & \text{for } |r_i| \leq \varepsilon \\ \varepsilon\left(|r_i| - \frac{1}{2}\varepsilon\right) & \text{otherwise} \end{cases}$$

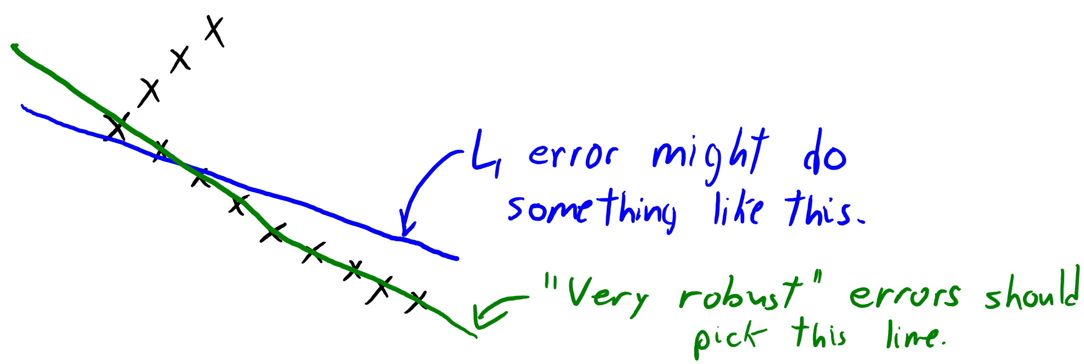


  - Note that 'h' is differentiable: h'(ε) = ε and h'(-ε) = -ε.
  - This 'f' is convex but setting ∇f(x) = 0 does not give a linear system.
    - But we can minimize the Huber loss using gradient descent.

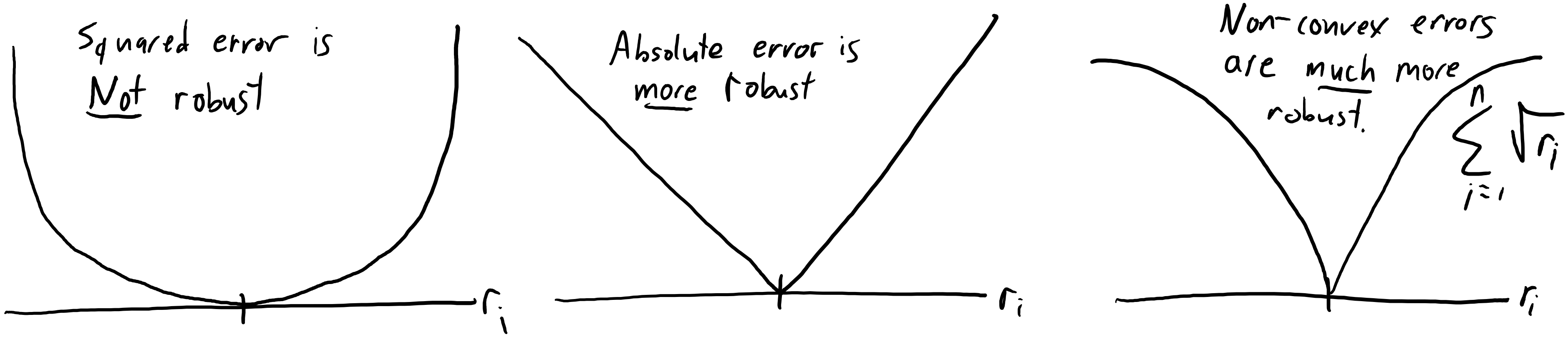
Very Robust Regression



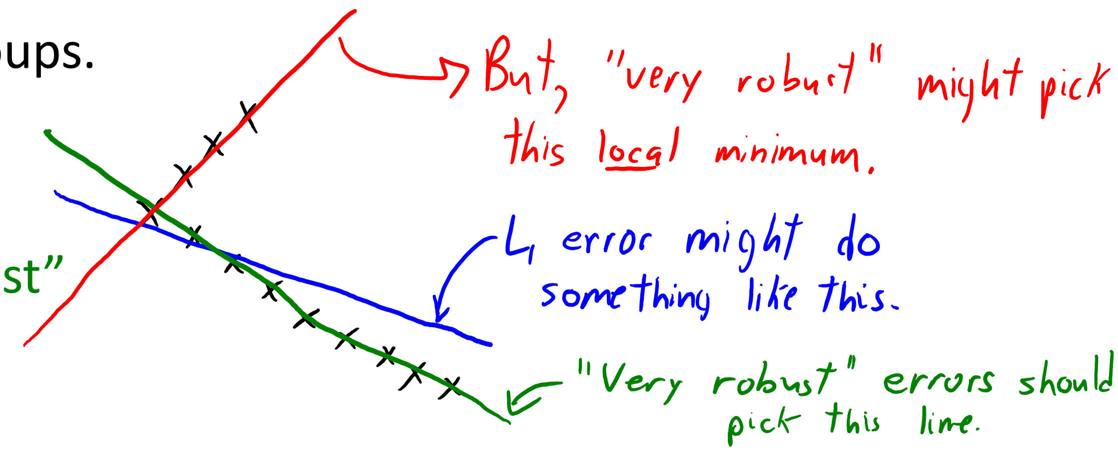
- Non-convex errors can be very robust:
  - Not influenced by outlier groups.



Very Robust Regression



- Non-convex errors can be very robust:
  - Not influenced by outlier groups.
  - But non-convex, so finding global minimum is hard.
  - Absolute value is "most robust" convex loss function.



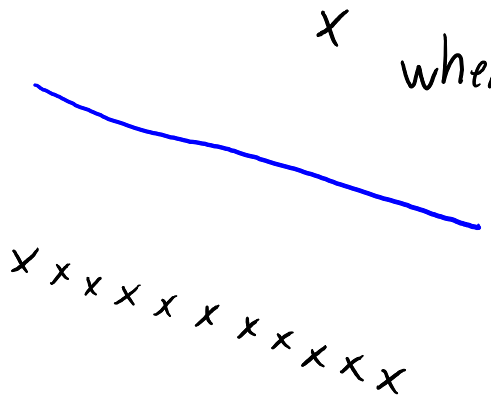
Motivation for Considering Worst Case

https://xkcd.com/937/

"Brittle" Regression

- What if you really care about getting the outliers right?
  - You want best performance on worst training example.
  - For example, if in worst case the plane can crash.
- In this case you could use something like the infinity-norm:

$$f(w) = \|Xw - y\|_\infty \quad \text{where } \|r\|_\infty = \max_i \{|r_i|\}$$



- Very sensitive to outliers ("brittle"), but worst case will be better.

Log-Sum-Exp Function

- As with the L_1-norm, the L_∞-norm is convex but non-smooth:
  - We can again use a smooth approximation and fit it with gradient descent.

- Convex and smooth approximation to max function is log-sum-exp function:

$$\max_i \{z_i\} \approx \log\left(\sum_i \exp(z_i)\right)$$

  - We'll use this several times in the course.
  - Notation alert: when I write "log" I always mean "natural" logarithm: log(e) = 1.

- Intuition behind log-sum-exp:
  - $\sum_i \exp(z_i) \approx \max_i \exp(z_i)$, as largest element is magnified exponentially (if no ties).
  - And notice that $\log(\exp(z_i)) = z_i$.

Log-Sum-Exp Function Examples

- Log-sum-exp function as smooth approximation to max:

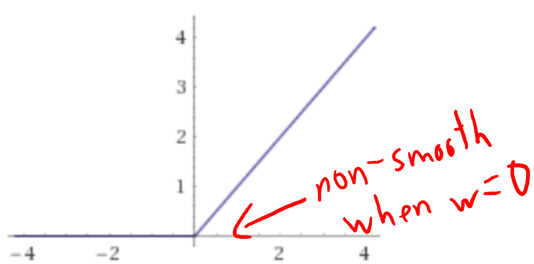
$$\max_i \{z_i\} \approx \log\left(\sum_i \exp(z_i)\right)$$

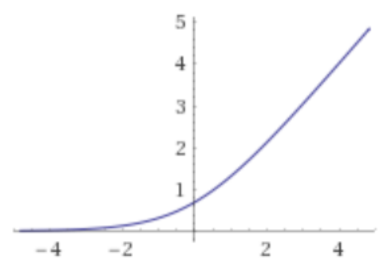
- If there aren't "close" values, it's really close to the max.

If $z_i = \{2, 20, 5, -100, 7\}$ then $\max_i \{z_i\} = 20$ and $\log\left(\sum_i \exp(z_i)\right) \approx 20.000002$

If $z_i = \{2, 20, 19.99, -100, 7\}$ then $\max_i \{z_i\} = 20$ and $\log\left(\sum_i \exp(z_i)\right) \approx 20.688160$

- Comparison of max{0,w} and smooth log(exp(0) + exp(w)):





Part 3 Key Ideas: Linear Models, Least Squares

- Focus of Part 3 is linear models:
  - Supervised learning where prediction is linear combination of features:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$$
$$= w^T x_i$$

- Regression:
  - Target y_i is numerical, testing ($\hat{y}_i$ == y_i) doesn't make sense.

Good fit that doesn't exactly pass through any point.

- Squared error: $\frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2$ or $\frac{1}{2}\|Xw - y\|^2$
  - Can find optimal 'w' by solving "normal equations".

Part 3 Key Ideas: Change of Basis, Gradient Descent

- Change of basis: replaces features x_i with non-linear transforms z_i:
  - Add a bias variable (feature that is always one).
  - Polynomial basis.
  - Other basis functions (logarithms, trigonometric functions, etc.).

- For large 'd' we often use gradient descent:
  - Iterations only cost O(nd).
  - Converges to a critical point of a smooth function.
  - For convex functions, it finds a global optimum.

Part 3 Key Ideas: Error Functions, Smoothing

- Error functions:
  - Squared error is sensitive to outliers.
  - Absolute (L_1) error and Huber error are more robust to outliers.
  - Brittle (L_∞) error is more sensitive to outliers.
- L_1 and L_∞ error functions are convex but non-differentiable:
  - Finding 'w' minimizing these errors is harder than squared error.
- We can approximate these with differentiable functions:
  - L_1 can be approximated with Huber.
  - L_∞ can be approximated with log-sum-exp.
- With these smooth (convex) approximations,
  we can find global optimum with gradient descent.

End of Scope for Midterm Material.

(we’re not done Part 3, but nothing after this point will be tested on the midterm)

Finding the "True" Model

- What if our goal is find the "true" model?
  - We believe that y_i really is a polynomial function of x_i.
  - We want to find the degree of the polynomial 'p'.

- Should we choose the 'p' with the lowest training error?
  - No, this will pick a 'p' that is way too large.
    (training error always decreases as you increase 'p')

Finding the "True" Model

- What if our goal is find the "true" model?
  - We believe that y_i really is a polynomial function of x_i.
  - We want to find the degree of the polynomial 'p'.

- Should we choose the 'p' with the lowest validation error?
  - This will also often choose a 'p' that is too large.

  - Even if true model has p=2, this is a special case of a degree-3 polynomial.
  - If 'p' is too big then we overfit, but might still get a lower validation error.
    - Another example of optimization bias.

Complexity Penalties

- There are a lot of "scores" people use to find the "true" model.
- Basic idea behind them: put a penalty on the model complexity.
  - Want to **fit the data and have a simple model**.
- For example, minimize training error plus the degree of polynomial.

Let $$Z_p = \begin{bmatrix} 1 & x_1 & (x_1)^2 & \cdots & (x_1)^p \\ 1 & x_2 & (x_2)^2 & \cdots & (x_2)^p \\ 1 & x_3 & (x_3)^2 & \cdots & (x_3)^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & (x_n)^2 & \cdots & (x_n)^p \end{bmatrix}$$

Find 'p' that minimizes:

$$\text{score}(p) = \underbrace{\frac{1}{2}\|Z_p v - y\|^2}_{\text{train error for best 'v' with this basis.}} + \underbrace{p}_{\text{degree of polynomial}}$$

  - If we use p=4, use "training error plus 4" as error.
- If two 'p' values have similar error, this prefers the smaller 'p'.

Choosing Degree of Polynomial Basis

- How can we optimize this score?

$$\text{score}(p) = \frac{1}{2}\|Z_p v - y\|^2 + p$$

  - Form Z_0, solve for 'v', compute score(0) = $\frac{1}{2}||Z_0 v - y||^2 + 0$.
  - Form Z_1, solve for 'v', compute score(1) = $\frac{1}{2}||Z_1 v - y||^2 + 1$.
  - Form Z_2, solve for 'v', compute score(2) = $\frac{1}{2}||Z_2 v - y||^2 + 2$.
  - Form Z_3, solve for 'v', compute score(3) = $\frac{1}{2}||Z_3 v - y||^2 + 3$.

  - Choose the degree with the lowest score.
    - "You need to decrease training error by at least 1 to increase degree by 1."

Information Criteria

- There are many scores, usually with the form:

$$\text{score}(p) = \frac{1}{2}\|Z_p v - y\|^2 + \lambda k$$

  - The value 'k' is the "number of estimated parameters" ("degrees of freedom").
    - For polynomial basis, we have k = (p+1).
  - The parameter $\lambda > 0$ controls how strong we penalize complexity.
    - "You need to decrease the training error by least λ to increase 'k' by 1".

- Using ($\lambda = 1$) is called Akaike information criterion (AIC).
- Other choices of λ give other criteria:
  - Mallow's C_p.
  - Adjusted R^2.
  - ANOVA-based model selection.

Choosing Degree of Polynomial Basis

- How can we optimize this score in terms of 'p'?

$$\text{score}(p) = \frac{1}{2}\|Z_p v - y\|^2 + \lambda k$$

  - Form Z_0, solve for 'v', compute score(0) = $\frac{1}{2}||Z_0v - y||^2 + \lambda$.
  - Form Z_1, solve for 'v', compute score(1) = $\frac{1}{2}||Z_1v - y||^2 + 2\lambda$.
  - Form Z_2, solve for 'v', compute score(2) = $\frac{1}{2}||Z_2v - y||^2 + 3\lambda$.
  - Form Z_3, solve for 'v', compute score(3) = $\frac{1}{2}||Z_3v - y||^2 + 4\lambda$.

  - So we need to improve by "at least λ" to justify increasing degree.
    - If λ is big, we'll choose a small degree. If λ is small, we'll choose a large degree.

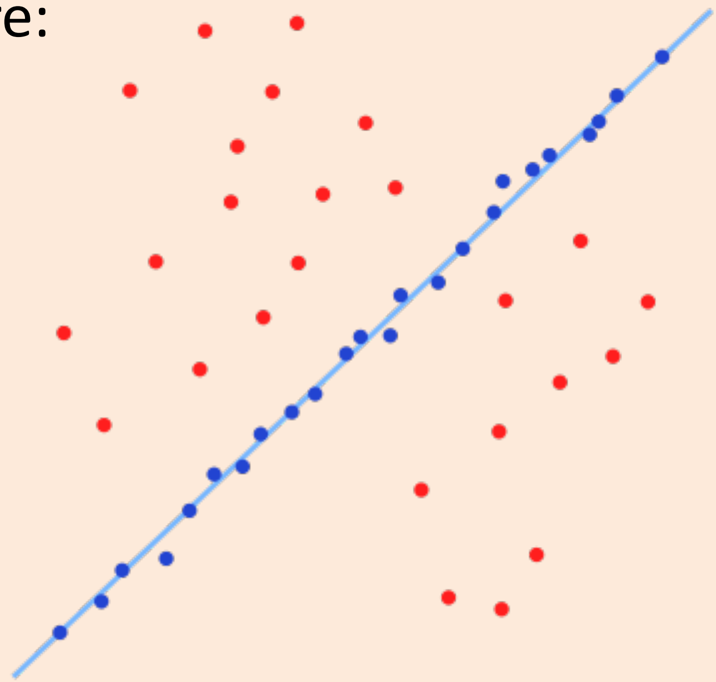
Summary

- Outliers in 'y' can cause problem for least squares.
- Robust regression using L1-norm is less sensitive to outliers.
- Brittle regression using Linf-norm is more sensitive to outliers.
- Smooth approximations:
  - Let us apply gradient descent to non-smooth functions.
  - Huber loss is a smooth approximation to absolute value.
  - Log-Sum-Exp is a smooth approximation to maximum.
- Information criteria are scores that penalize number of parameters.
  - When we want to find the "true" model.

- Next time:
  - Can we find the "true" features?

Random Sample Consensus (RANSAC)

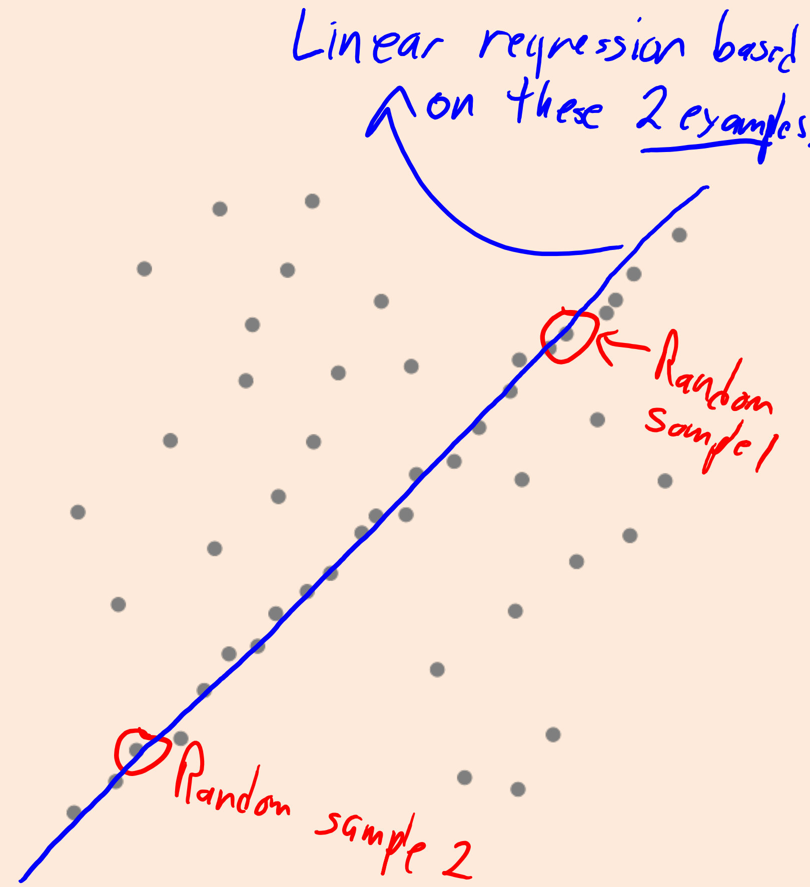
- In computer vision, a widely-used generic framework for robust fitting is random sample consensus (RANSAC).
- This is designed for the scenario where:
  - You have a large number of outliers.
  - Majority of points are "inliers":
    it's really easy to get low error on them.



https://en.wikipedia.org/wiki/Random_sample_consensus

Random Sample Consensus (RANSAC)

- RANSAC:
  - Sample a small number of training examples.
    - Minimum number needed to fit the model.
    - For linear regression with 1 feature, just 2 examples.
  - Fit the model based on the samples.
    - Fit a line to these 2 points.
    - With 'd' features, you'll need 'd+1' examples.
  - Test how many points are fit well based on the model.
  - Repeat until we find a model that fits at least the expected number of "inliers".
- You might then re-fit based on the estimated "inliers".



https://en.wikipedia.org/wiki/Random_sample_consensus

Log-Sum-Exp for Brittle Regression

- To use log-sum-exp for brittle regression:

$$\|Xw - y\|_\infty = \max_i \{|w^T x_i - y_i|\}$$

$$= \max_i \{\max\{w^T x_i - y_i, y_i - w^T x_i\}\} \quad \text{since } |z| = \max\{z, -z\}$$

$$= \log\left(\sum_{i=1}^n \exp(w^T x_i - y_i) + \sum_{i=1}^n \exp(y_i - w^T x_i)\right)$$

using log-sum-exp to approximate "max" over $2n$ terms.

Log-Sum-Exp Numerical Trick

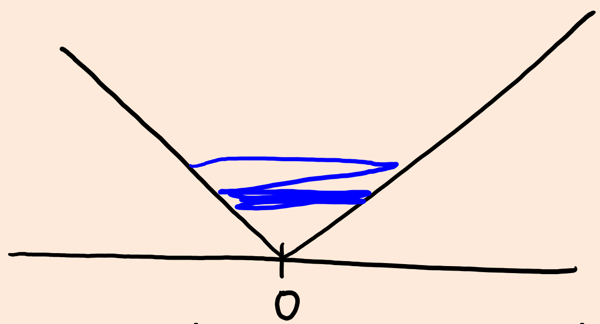
- Numerical problem with log-sum-exp is that $\exp(z_i)$ might overflow.
  - For example, exp(100) has more than 40 digits.
- Implementation 'trick': Let $\beta = \max_i \{z_i\}$

$$\log\left(\sum_i \exp(z_i)\right) = \log\left(\sum_i \exp(z_i - \beta + \beta)\right)$$
$$= \log\left(\sum_i \exp(z_i - \beta)\exp(\beta)\right)$$
$$= \log\left(\exp(\beta)\sum_i \exp(z_i - \beta)\right)$$
$$= \log(\exp(\beta)) + \log\left(\sum_i \exp(z_i - \beta)\right)$$
$$= \beta + \log\left(\sum_i \underbrace{\exp(z_i - \beta)}_{\leq 1}\right)$$

so no overflow

Gradient Descent for Non-Smooth?

- "You are unlikely to land on a non-smooth point, so gradient descent should work for non-smooth problems?"
  - Consider just trying to minimize the absolute value function:



  - Norm(gradient) is constant when not at 0, so unless you are lucky enough to hit exactly 0, you will just bounce back and forth forever.
  - We didn't have this problem for smooth functions, since the gradient gets smaller as you approach a minimizer.
  - You could fix this problem by making the step-size slowly go to zero, but you need to do this carefully to make it work, and the algorithm gets much slower.

Gradient Descent for Non-Smooth?

- Counter-example from Bertsekas' "Nonlinear Programming" where gradient descent for a non-smooth convex problem does not converge to a minimum.

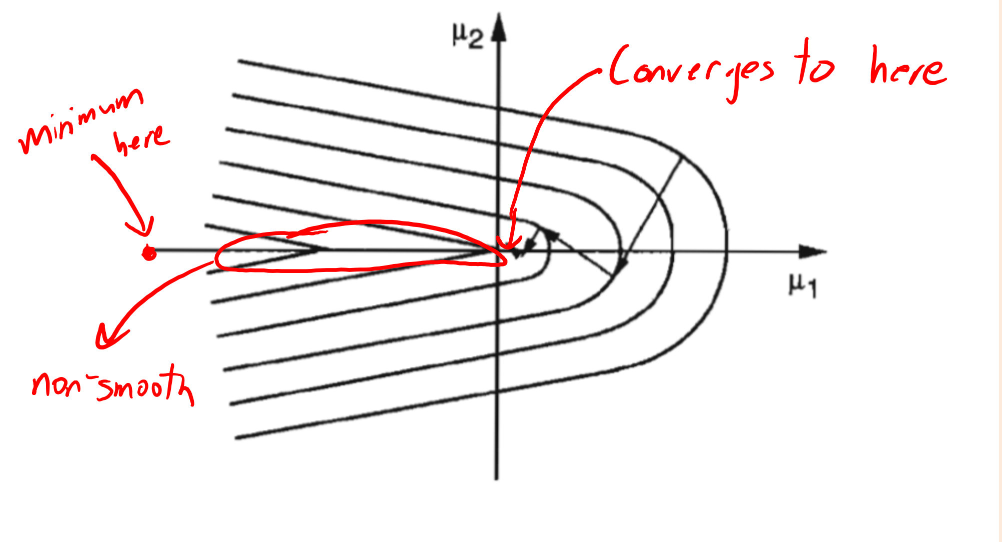


Figure 6.3.8. Contours and steepest ascent path for the function of Exercise 6.3.8.

(even though function is convex)