

CPSC 340: Machine Learning and Data Mining

Robust Regression

Fall 2021

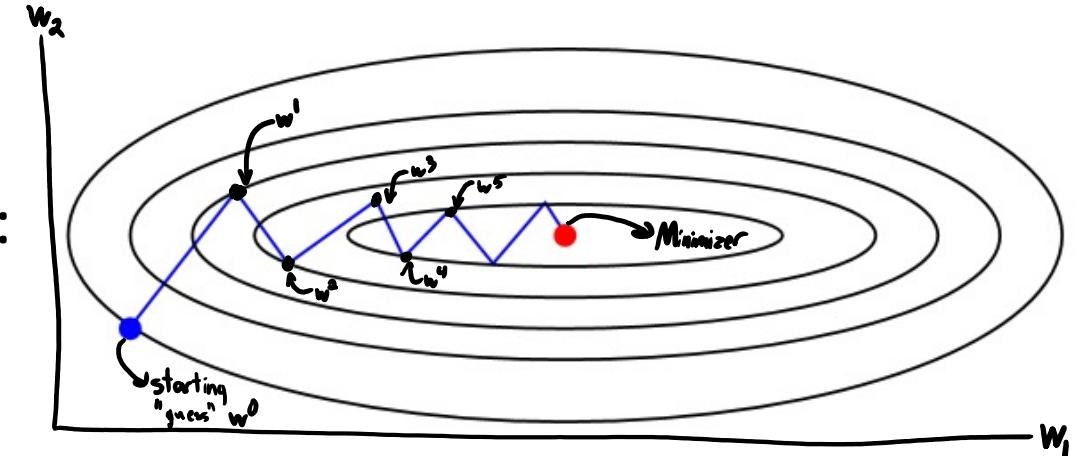
Admin

- Midterm
 - Thu Oct 21 from 6:00-7:30pm
 - You will have 85 minutes in that 90-minute window
 - Covers assignments 1-3, lectures up to & including today
 - We have booked SCRF 100 for those who'd like a quiet space to work
- Mid-course survey
 - <https://bit.ly/340-survey2>
 - Please take a couple minutes now to complete the survey. Thanks!
- Reminder about collaboration policies for assignments

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 $\nabla f(w) = 0$ 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 (Easy Way)

- 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

bonus!

Convexity in Higher Dimensions

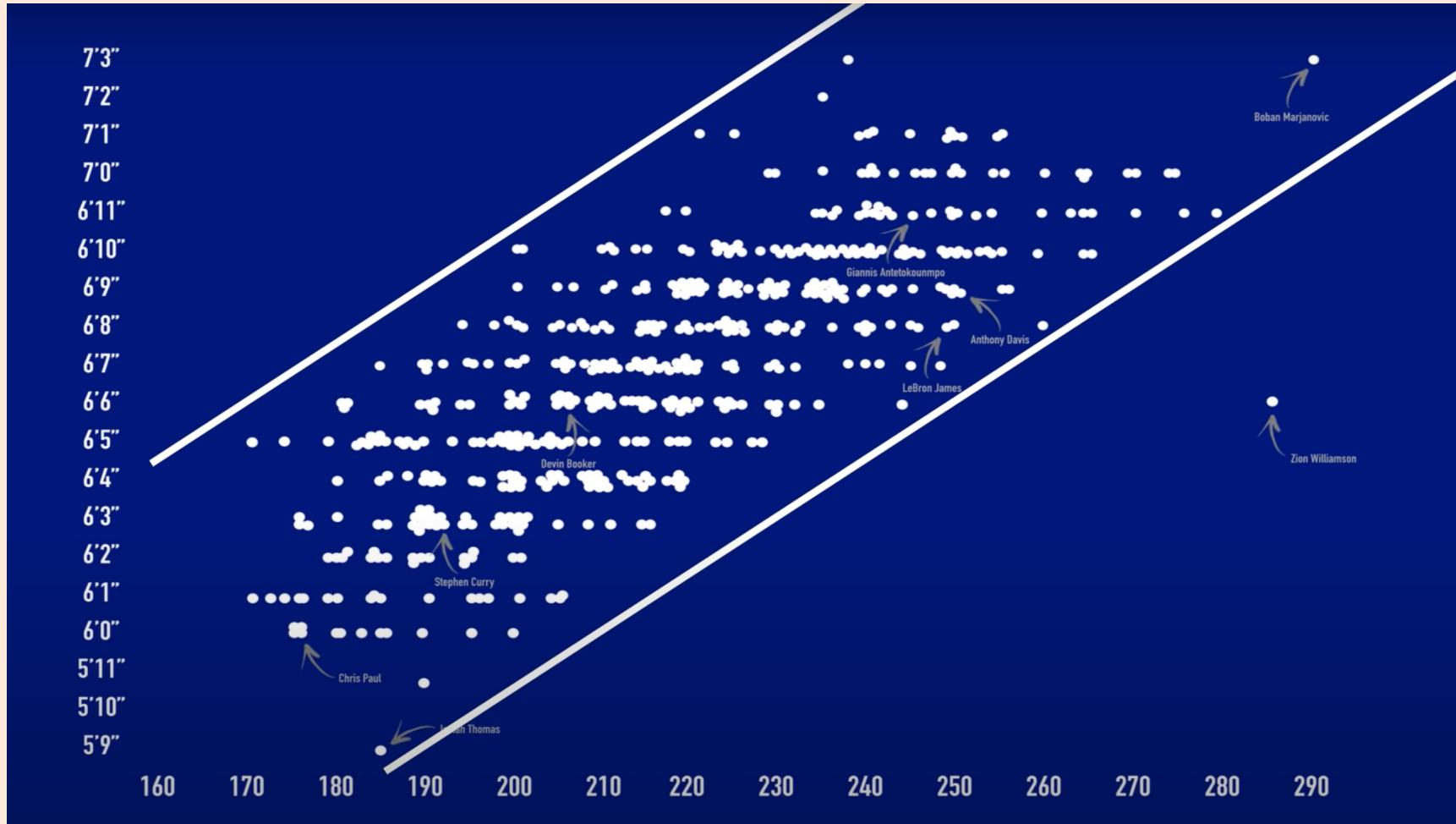
- Twice-differentiable ‘d’-variable function is **convex** iff:
 - Eigenvalues of Hessian $\nabla^2 f(w)$ are non-negative for all ‘w’.
- True for least squares where $\nabla^2 f(w) = X^T X$ for all ‘w’.
 - See bonus slides for why $X^T X$ has non-negative eigenvalues.
- Unfortunately, sometimes it is hard to show convexity this way.
 - Usually **easier** to just use some of the rules as we did on the last slide.

(pause)

bonus!

Least Squares with Outliers

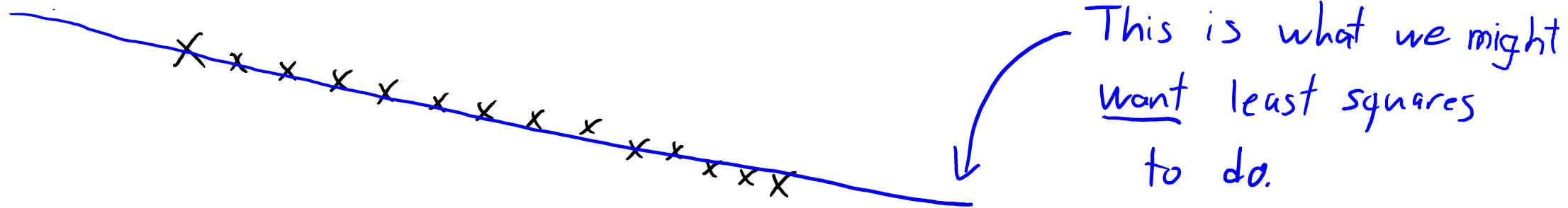
- Height vs. weight of NBA players:



Least Squares with Outliers

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

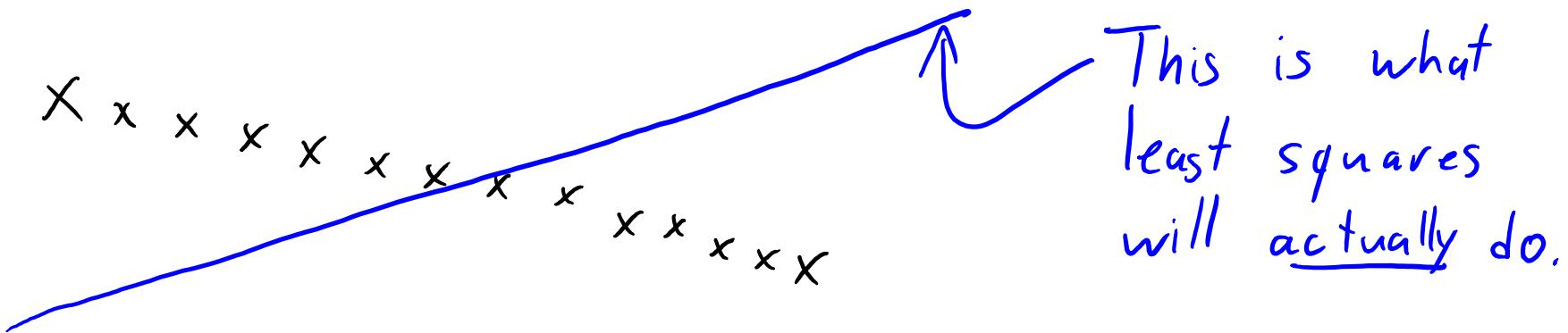
$x \leftarrow$ "outlier" that doesn't follow trend



Least Squares with Outliers

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

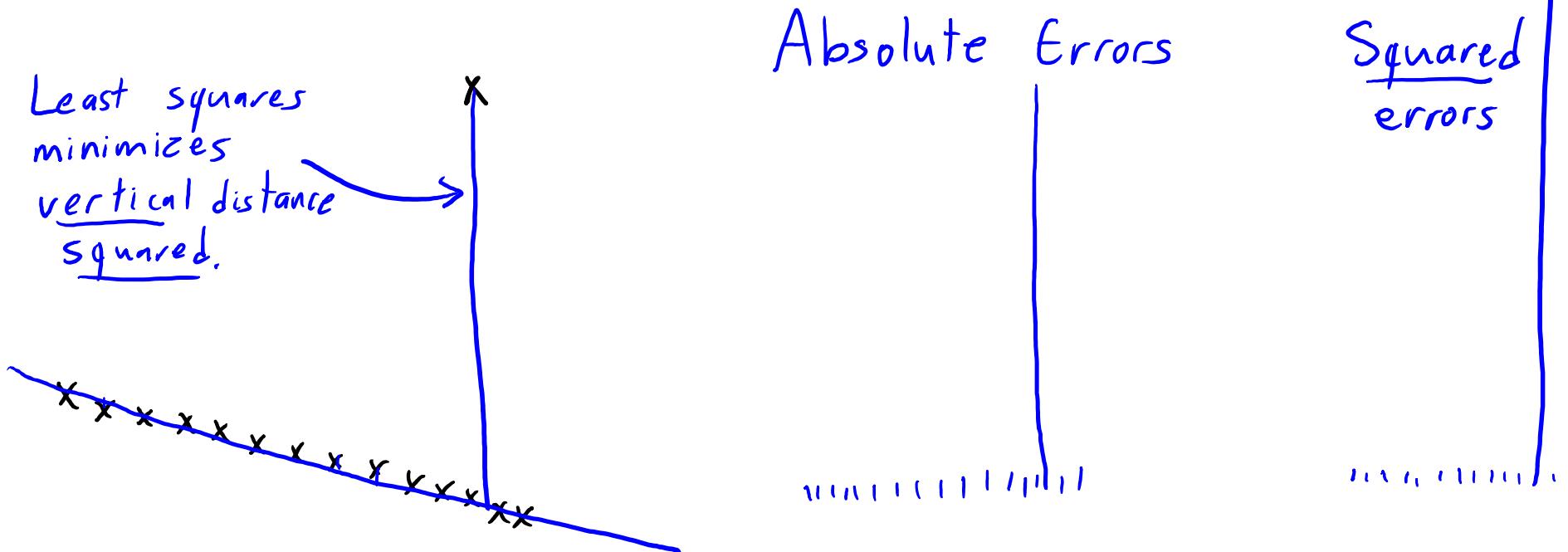
$x \leftarrow$ "outlier" that doesn't follow trend



- Least squares is very sensitive to outliers.

Least Squares with Outliers

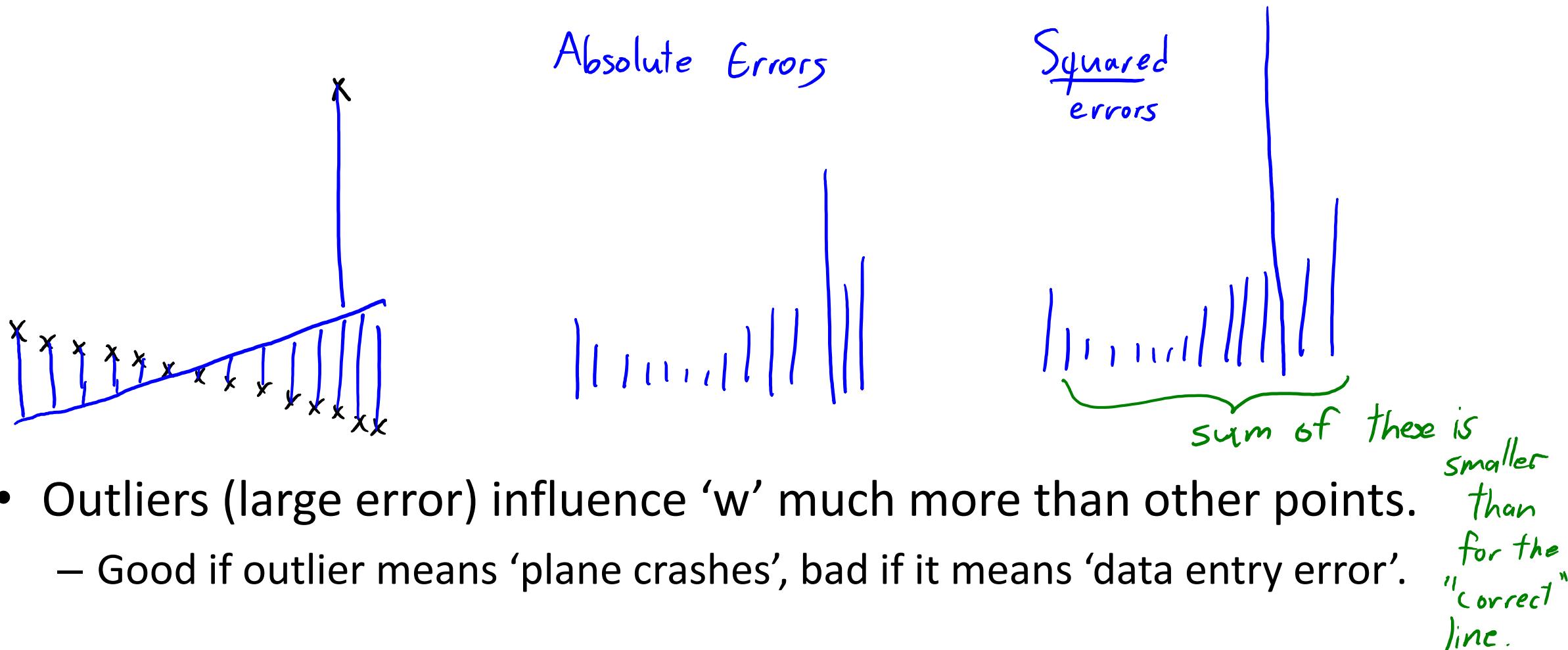
- Squaring error shrinks small errors, and **magnifies large errors**:



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

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'.

Robust Regression

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

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

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

Least squares:

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

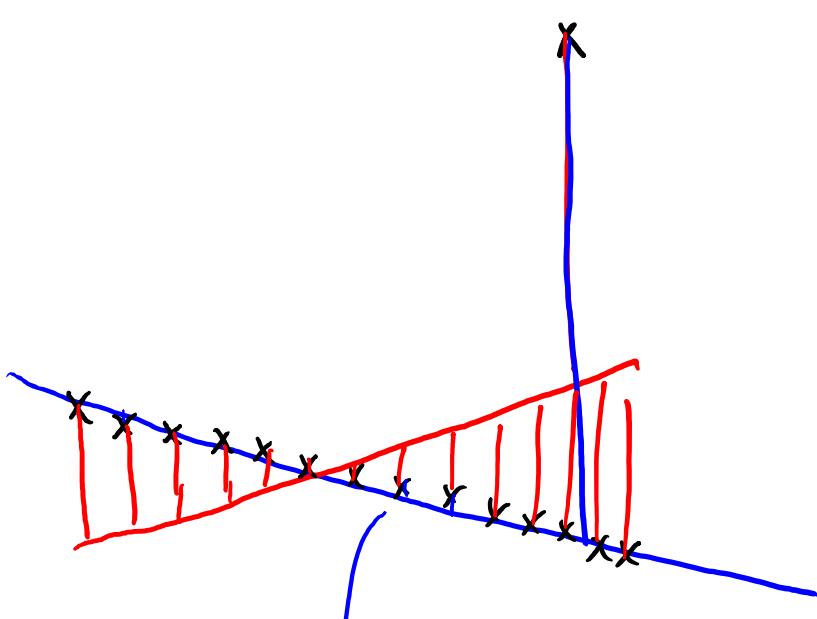
Least absolute error:

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

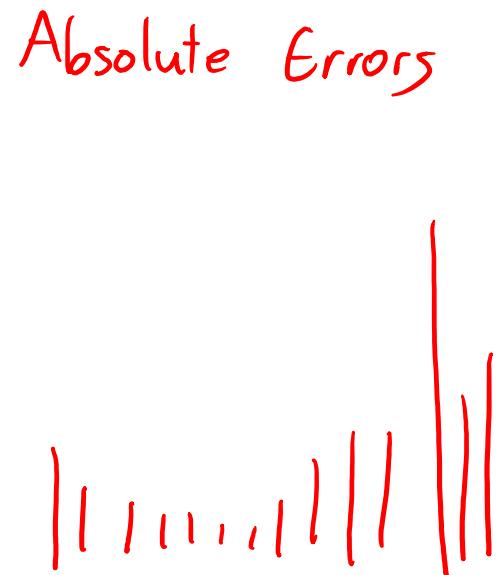
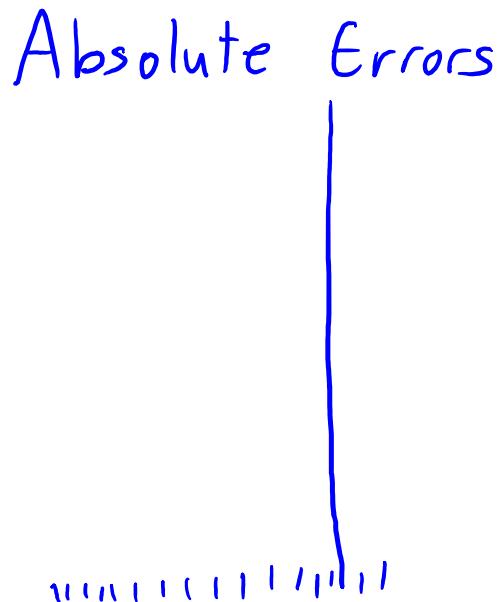
$$\begin{aligned} & \sum_{i=1}^n |w^\top x_i - y_i| \\ &= \sum_{i=1}^n |r_i| = \|r\|_1 \\ &= \|X_w - y\|_1 \end{aligned}$$

Least Squares with Outliers

- Absolute error is more robust to outliers:

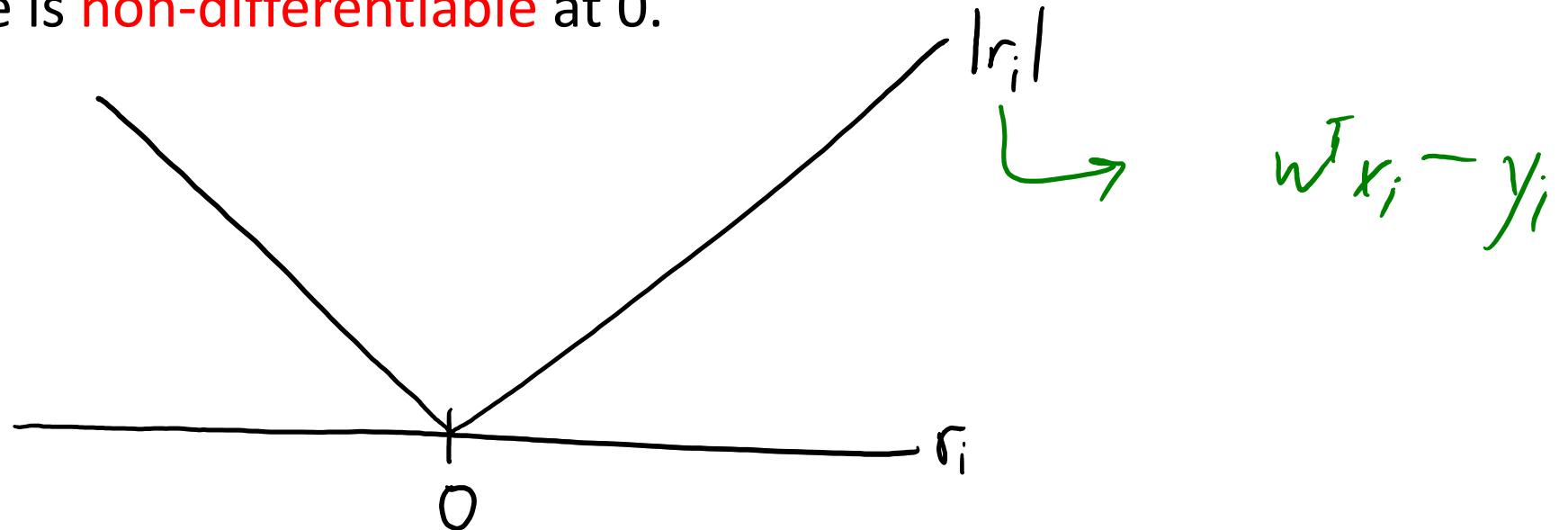


Linear model ' w ' minimizing $f(w) = \|Xw - y\|_1 = \sum_{i=1}^n |w^T x_i - y_i|$



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.



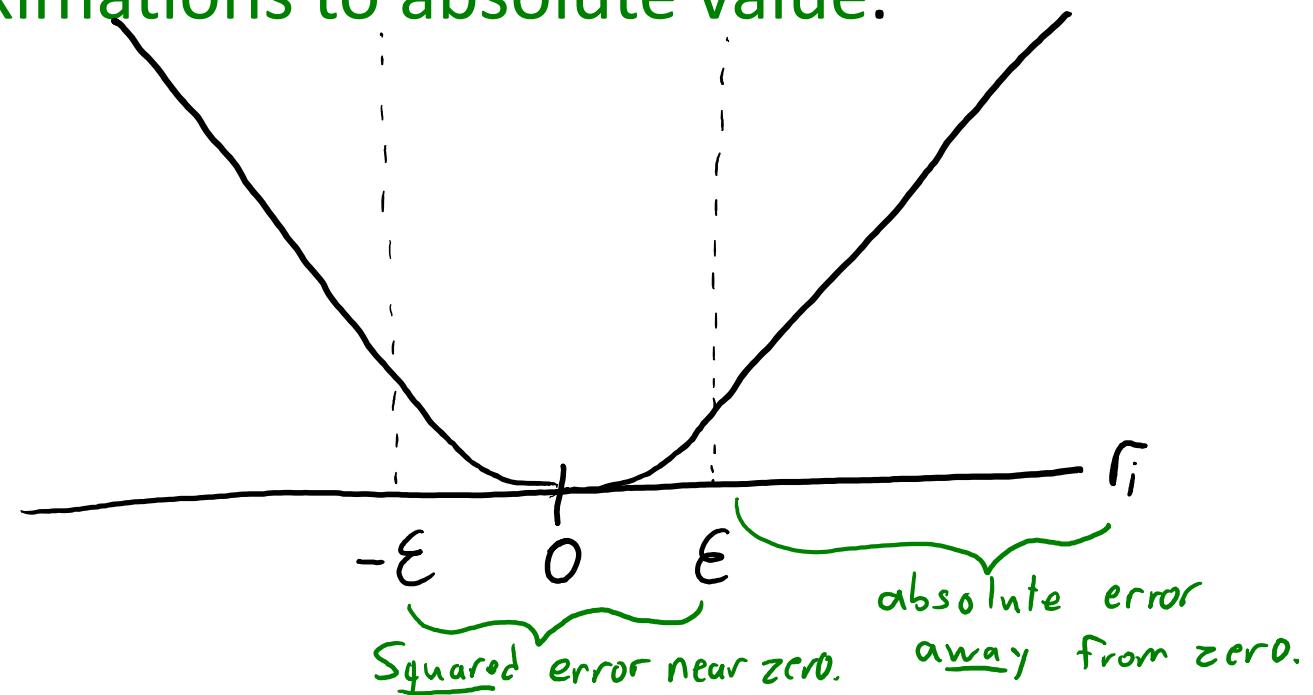
- Generally, harder to minimize non-smooth than smooth functions.
 - Unlike smooth functions, the gradient may not get smaller near a minimizer.
- To apply gradient descent, we'll use a smooth approximation.

Smooth Approximations to the L1-Norm

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

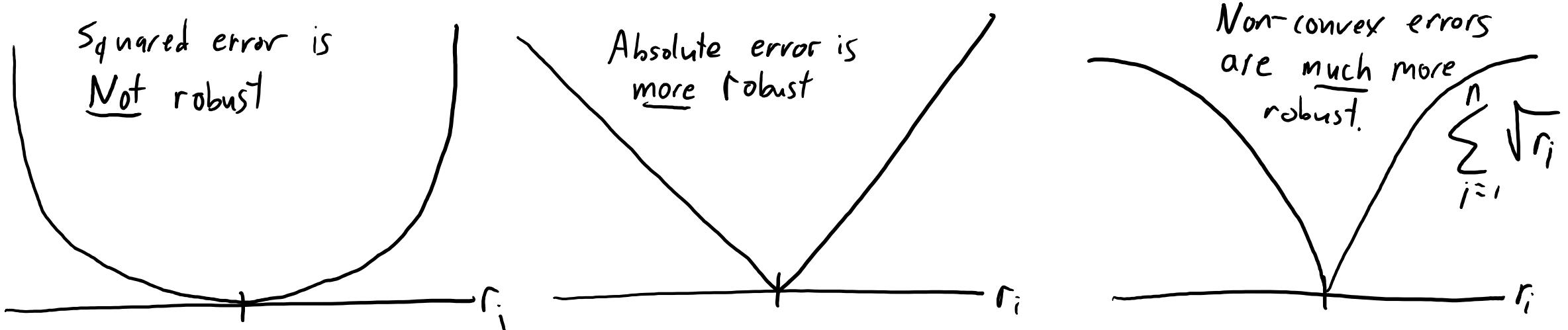
$$f(w) = \sum_{i=1}^n h(w^T x_i - y_i)$$

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

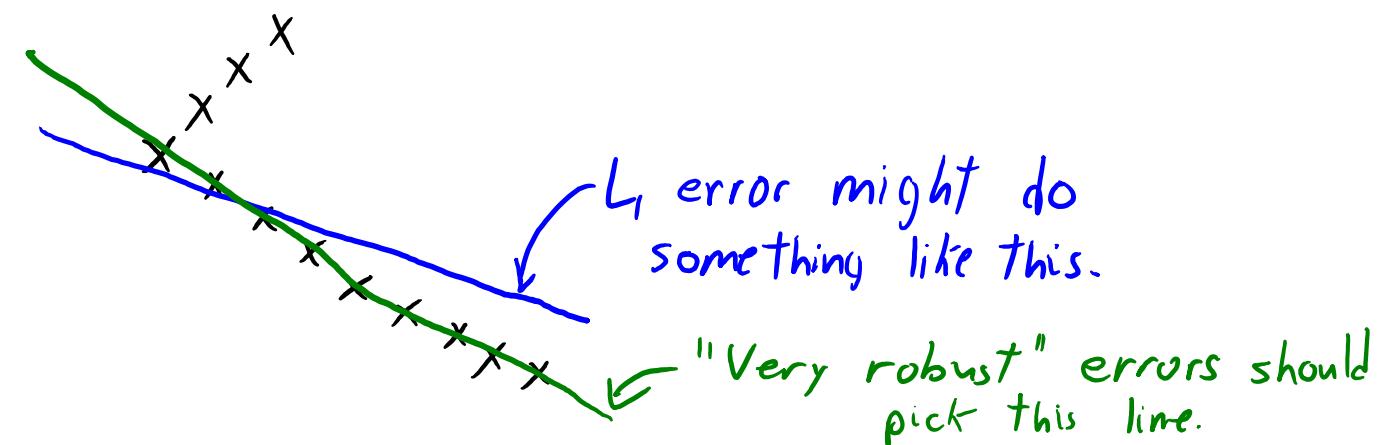


- Note that 'h' is differentiable: $h'(\varepsilon) = \varepsilon$ and $h'(-\varepsilon) = -\varepsilon$.
- This 'f' is convex but setting $\nabla f(x) = 0$ does not give a linear system.
 - But we can minimize the Huber loss using gradient descent.

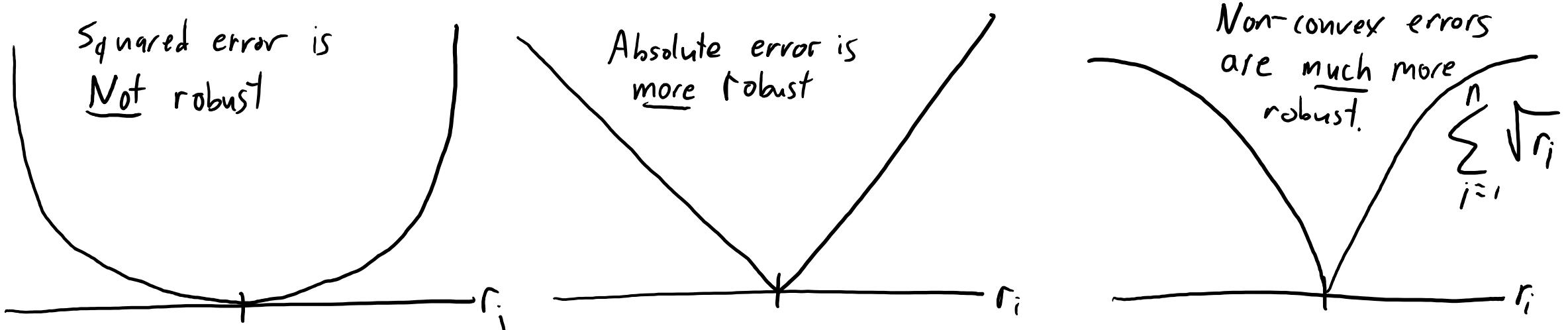
Very Robust Regression



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

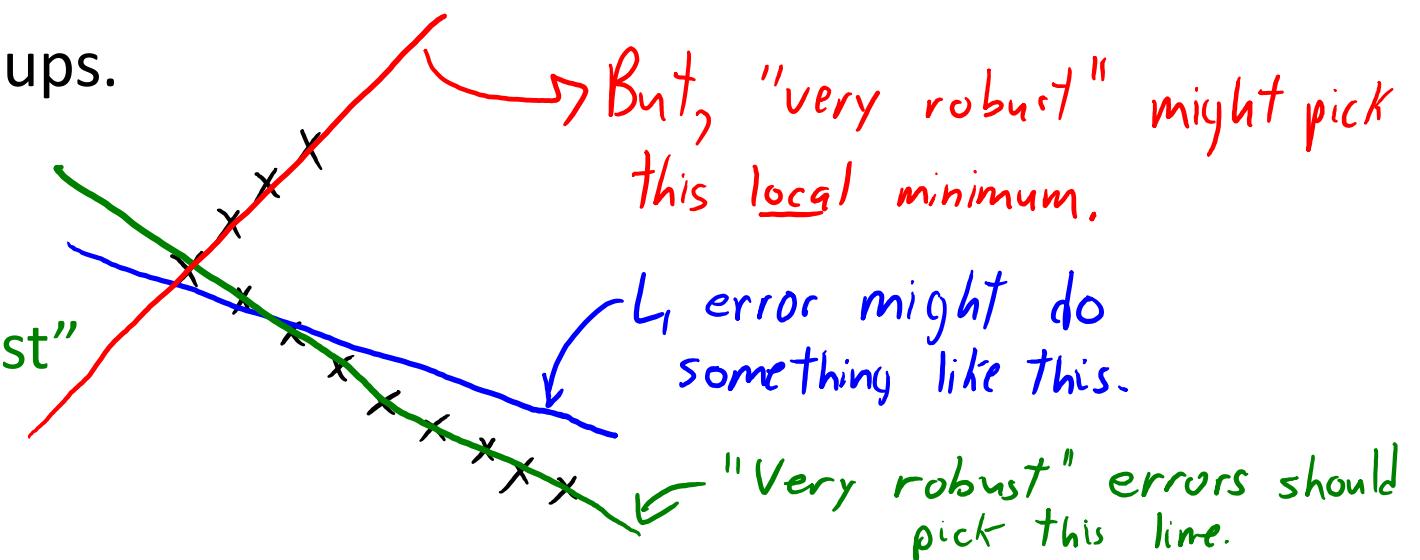


Very Robust Regression



- 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.



bonus!

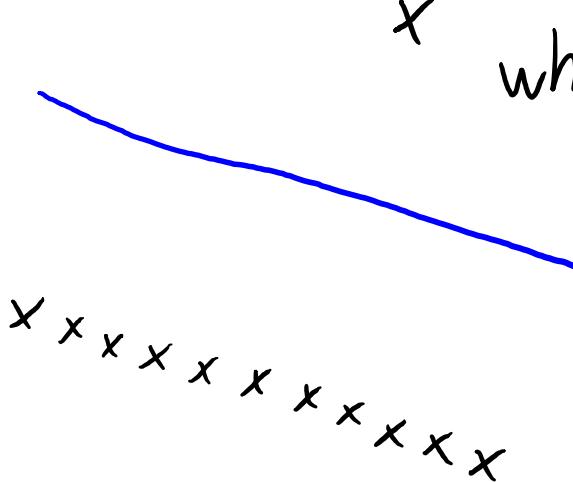
Motivation for Modeling Outliers



- What if the “outlier” is the only non-male person in your dataset?
 - Do you want to be robust to the outlier?
 - Will the model work for everyone if it has good average case performance?

“Brittle” Regression

- What if you really care about **getting the outliers right?**
 - You want to **minimize size of worst error** across examples.
 - 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 minimizes highest errors.

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:

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

- We'll use this several times in the course.
- Notation reminder: 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:

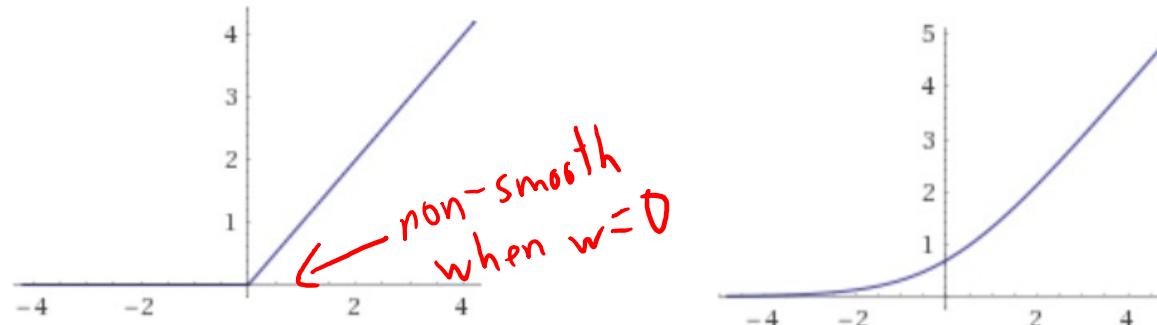
$$\max_i \{z_i\} \approx \log(\sum_i \exp(z_i))$$

- 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 $\log(\sum_i \exp(z_i)) \approx 20.066602$

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

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



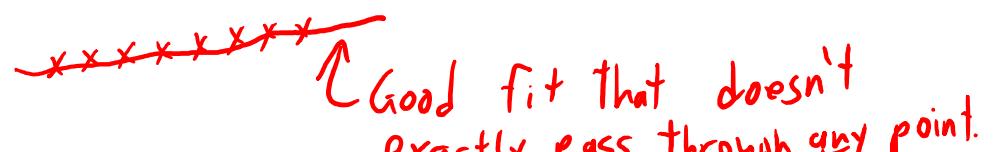
Part 3 Key Ideas: Linear Models, Least Squares

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

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

- **Regression**:

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

- **Squared error**: $\frac{1}{2} \sum_{i=1}^n (\hat{y}_i - y_i)^2$ or $\frac{1}{2} \|x_w - y\|^2$
- Good fit that doesn't exactly pass through any point.
- 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**.

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

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

train error for best ' v ' with this basis. 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?

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

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

$$\text{Score}(\beta) = \frac{1}{2} \|z_{\beta} - y\|^2 + \lambda k$$

- 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 (not necessarily integer) give other criteria:
 - Mallow’s C_p .
 - Adjusted R^2 .
 - ANOVA-based model selection.

bonus!

Naming something after yourself without being gauche

Akaike Information Criterion



P.S. When introducing AIC, Akaike called it An Information Criterion. When introducing WAIC, Watanabe called it the Widely Applicable Information Criterion. Aki and I are hoping to come up with something called the Very Good Information Criterion.

Watanabe-Akaike Info. Criterion



Aki Ventari

Andrew Gelman

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

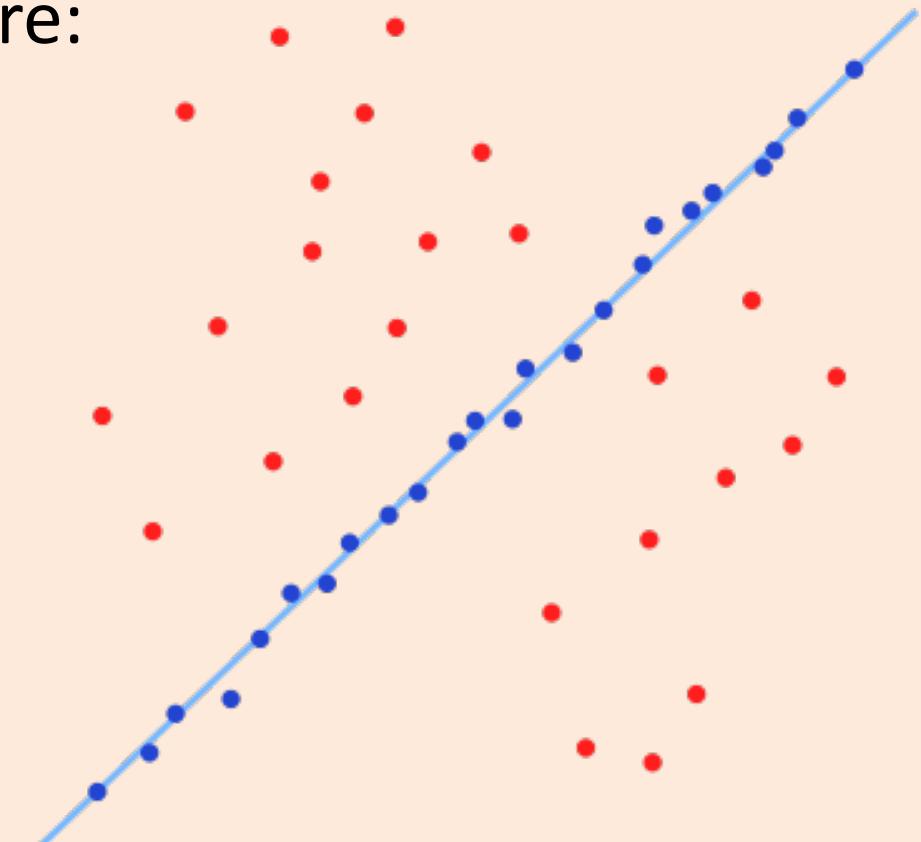
Summary

- 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?

bonus!

Random Sample Consensus (RANSAC)

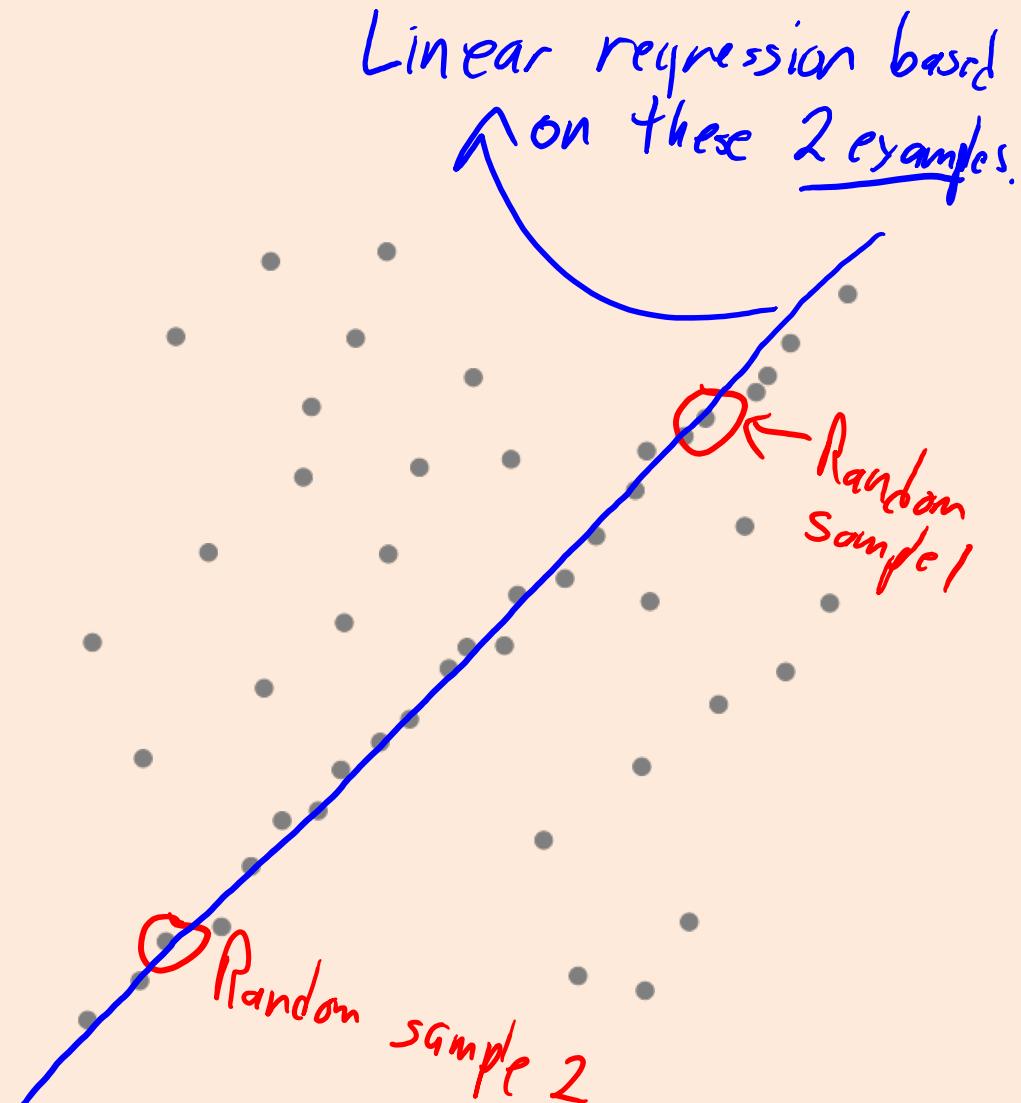
- In computer vision, a widely-used generic framework for robust fitting is **random sample consensus (RANSAC)**.
- This is designed for the scenario where:
 - You have a large number of outliers.
 - Majority of points are “inliers”: it’s really easy to get low error on them.



bonus!

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”.



bonus!

Log-Sum-Exp for Brittle Regression

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

$$\begin{aligned}\|x_w - y\|_\infty &= \max_i \{|w^T x_i - y_i|\} \\ &= \max_i \left\{ \max \left\{ w^T x_i - y_i, y_i - w^T x_i \right\} \right\} \quad \text{since } |z| = \max\{z, -z\} \\ &= \log \left(\sum_{i=1}^n \exp(w^T x_i - y_i) + \sum_{i=1}^n \exp(y_i - w^T x_i) \right) \quad \text{using log-sum-exp} \\ &\quad \text{to approximate} \\ &\quad \text{"max" over } 2n \text{ terms.}\end{aligned}$$

bonus!

Log-Sum-Exp Numerical Trick

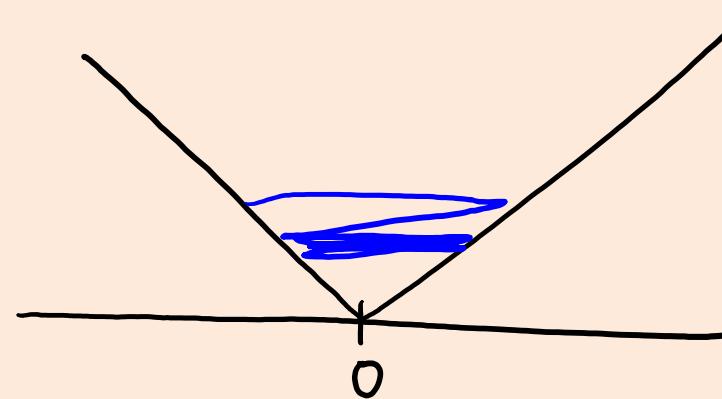
- Numerical problem with log-sum-exp is that $\exp(z_i)$ might overflow.
 - For example, $\exp(100)$ has more than 40 digits.
- Implementation ‘trick’: Let $\beta = \max_i \{z_i\}$

$$\begin{aligned}\log\left(\sum_i \exp(z_i)\right) &= \log\left(\sum_i \exp(z_i - \beta + \beta)\right) \\ &= \log\left(\sum_i \exp(z_i - \beta) \exp(\beta)\right) \\ &= \log(\exp(\beta)) \sum_i \exp(z_i - \beta) \\ &= \log(\exp(\beta)) + \log\left(\sum_i \exp(z_i - \beta)\right) \\ &= \beta + \log\left(\sum_i \exp(z_i - \beta)\right) \xrightarrow{\text{so no overflow}} \leq 1\end{aligned}$$

bonus!

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.

bonus!

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.

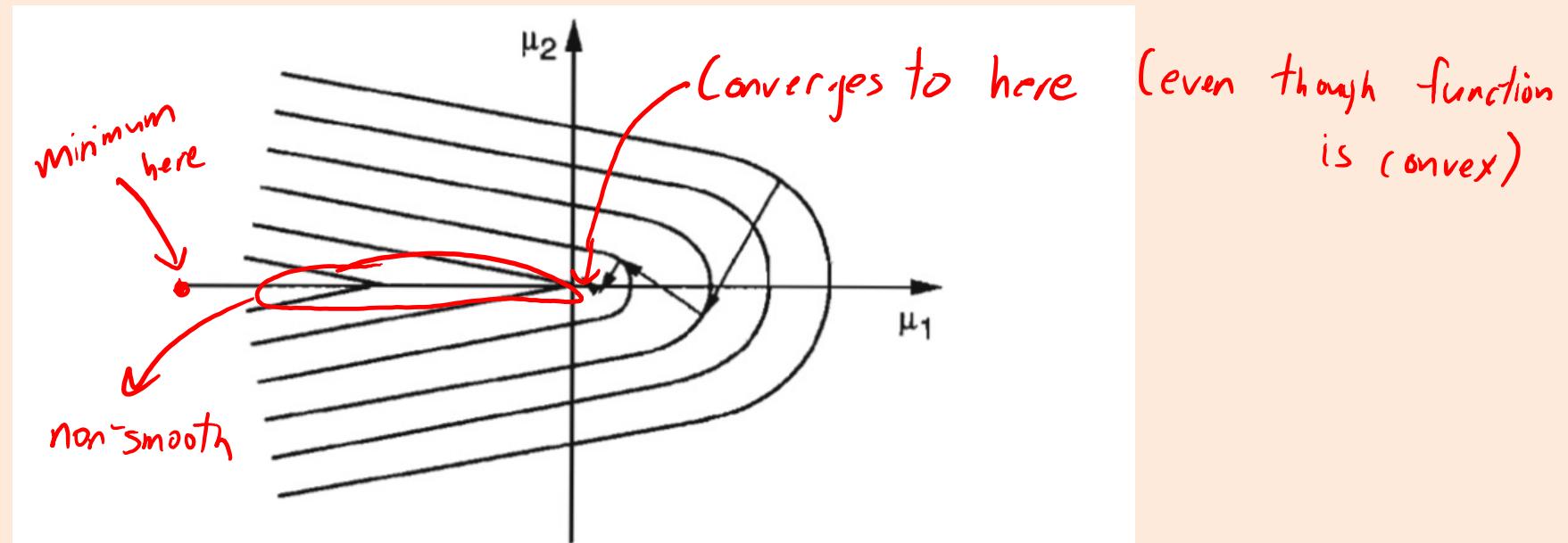


Figure 6.3.8. Contours and steepest ascent path for the function of Exercise 6.3.8.

bonus!

Example: Convexity of Linear Regression (Hard Way)

- Consider linear regression objective with squared error:

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

- Twice-differentiable 'f' is convex if $\nabla^2 f(x)$ has eigenvalues ≥ 0 .
 - This is equivalent to saying $v^T \nabla^2 f(x)v \geq 0$ for all vectors v .
- The Hessian for least squares is $\nabla^2 f(x) = X^T X$.
 - See notes on Gradients and Hessians of quadratics on webpage.
- We have: $v^T \nabla^2 f(w)v = v^T X^T X v = (Xv)^T (Xv) = \|Xv\|^2 \geq 0$ (because norms are ≥ 0)

So it's convex