# CPSC 340: Machine Learning and Data Mining

Robust Regression

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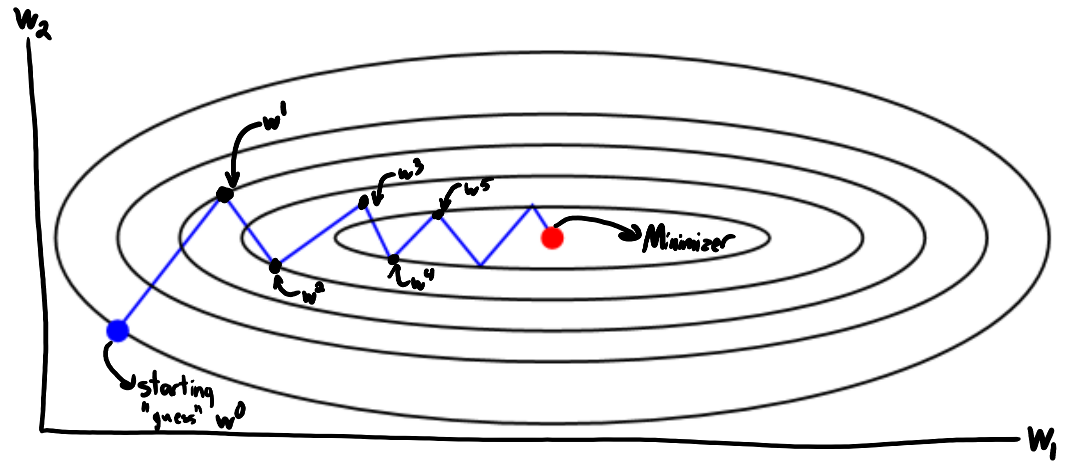
University of British Columbia, Fall 2022
https://www.students.cs.ubc.ca/~cs-340

# 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 (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 <u>linear</u> function ('d' inputs, 'n' outputs)

Let $g(r) = \|r\|^2$, which is <u>convex</u> because it's a squared norm.

Then $f(w) = g(h(w))$, which is <u>convex</u> because it's a <u>convex</u> function composed with a <u>linear</u> 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’.

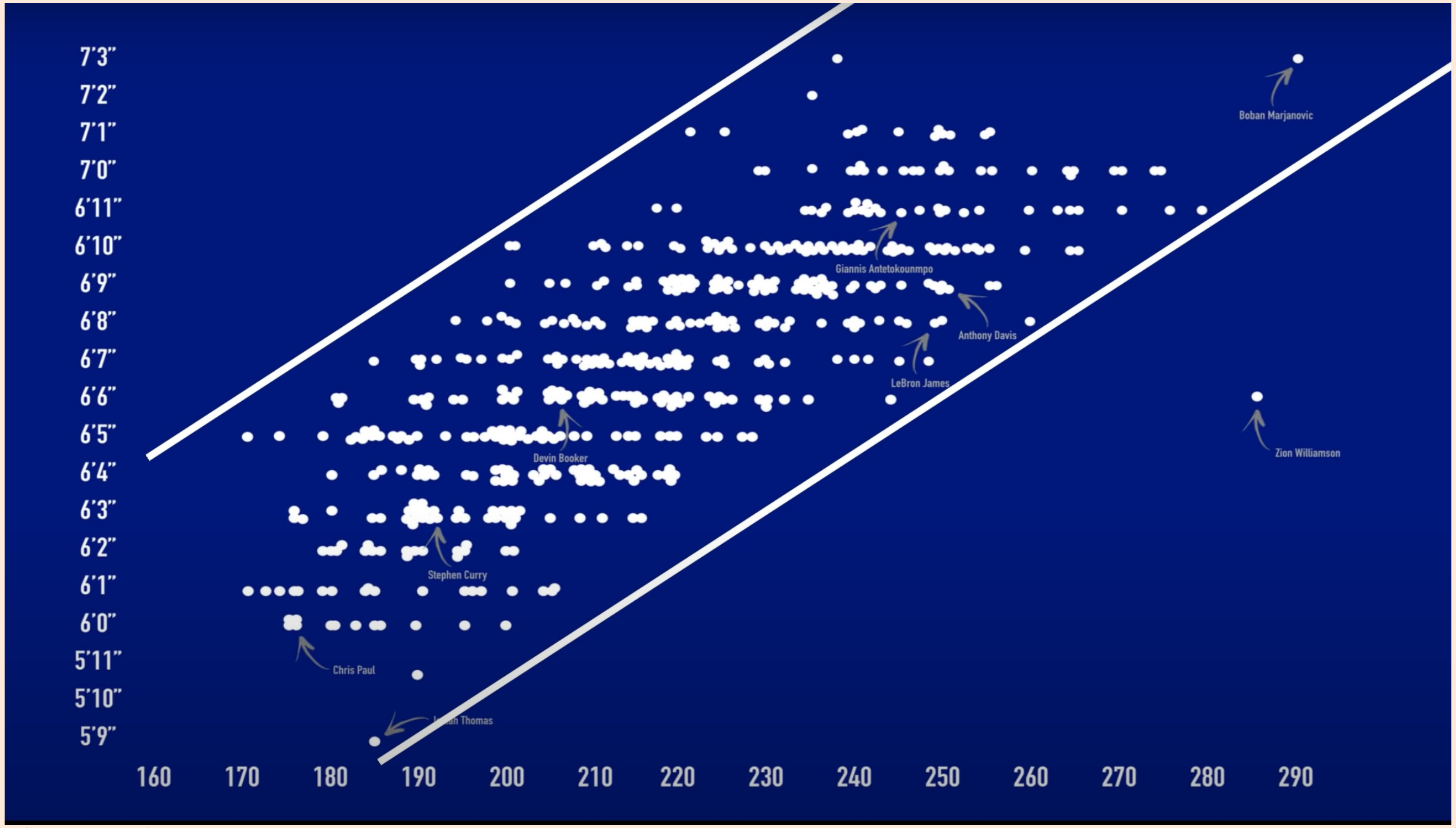
- True for least squares where $\nabla^2 f(w) = X^T X$ for all ‘w’.
  - See bonus slides for why $X^T X$ has non-negative eigenvalues.

- 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.

## Next Topic: Robust Regression

# Least Squares with Outliers

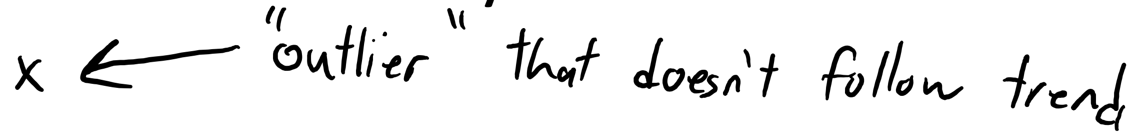
- Height vs. weight of NBA players:

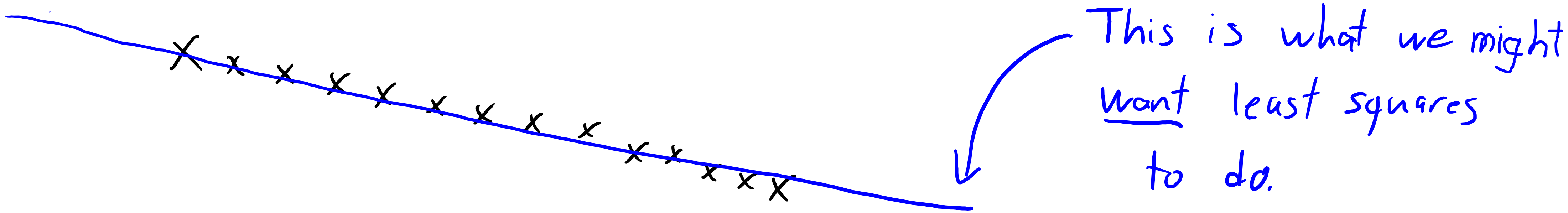


https://www.youtube.com/watch?v=i4eYWl1ewFo

## Least Squares with Outliers

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

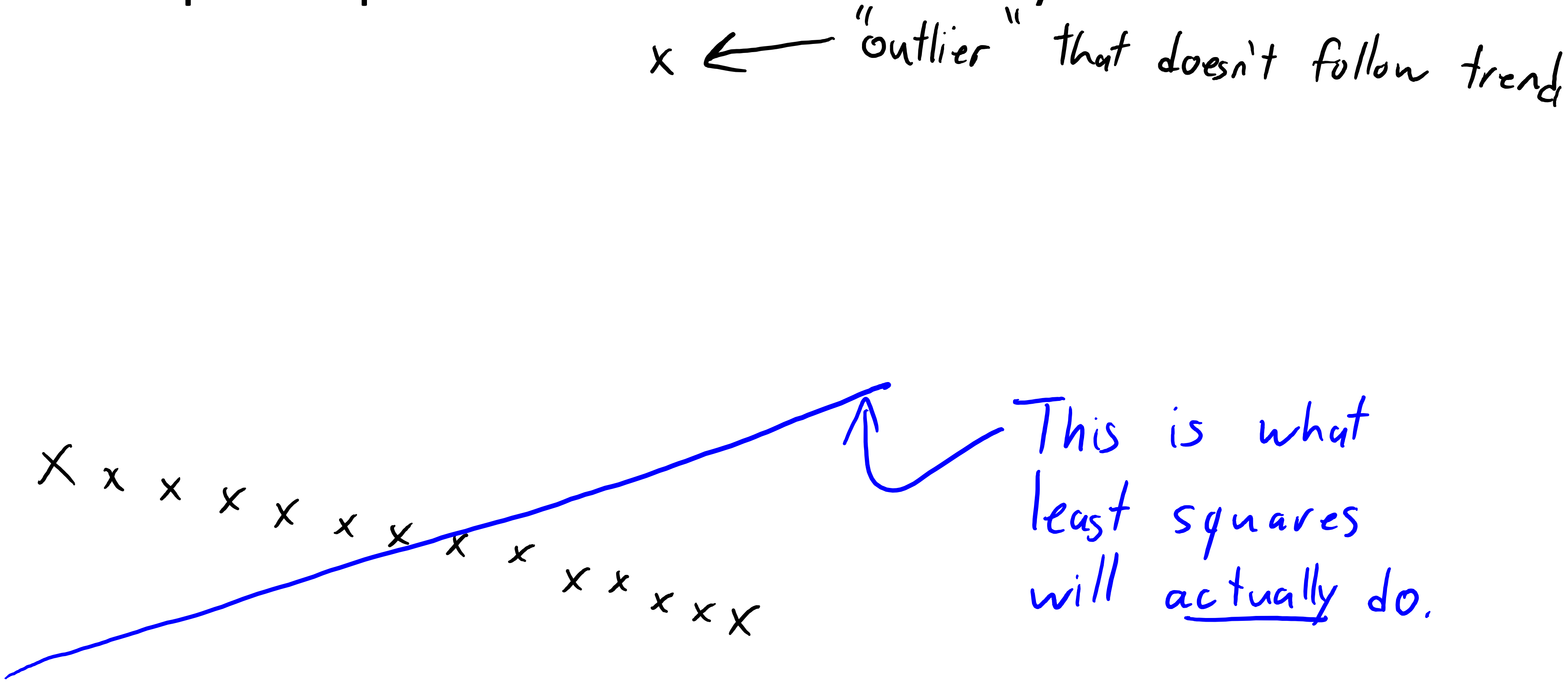




http://setosa.io/ev/ordinary-least-squares-regression

# Least Squares with Outliers

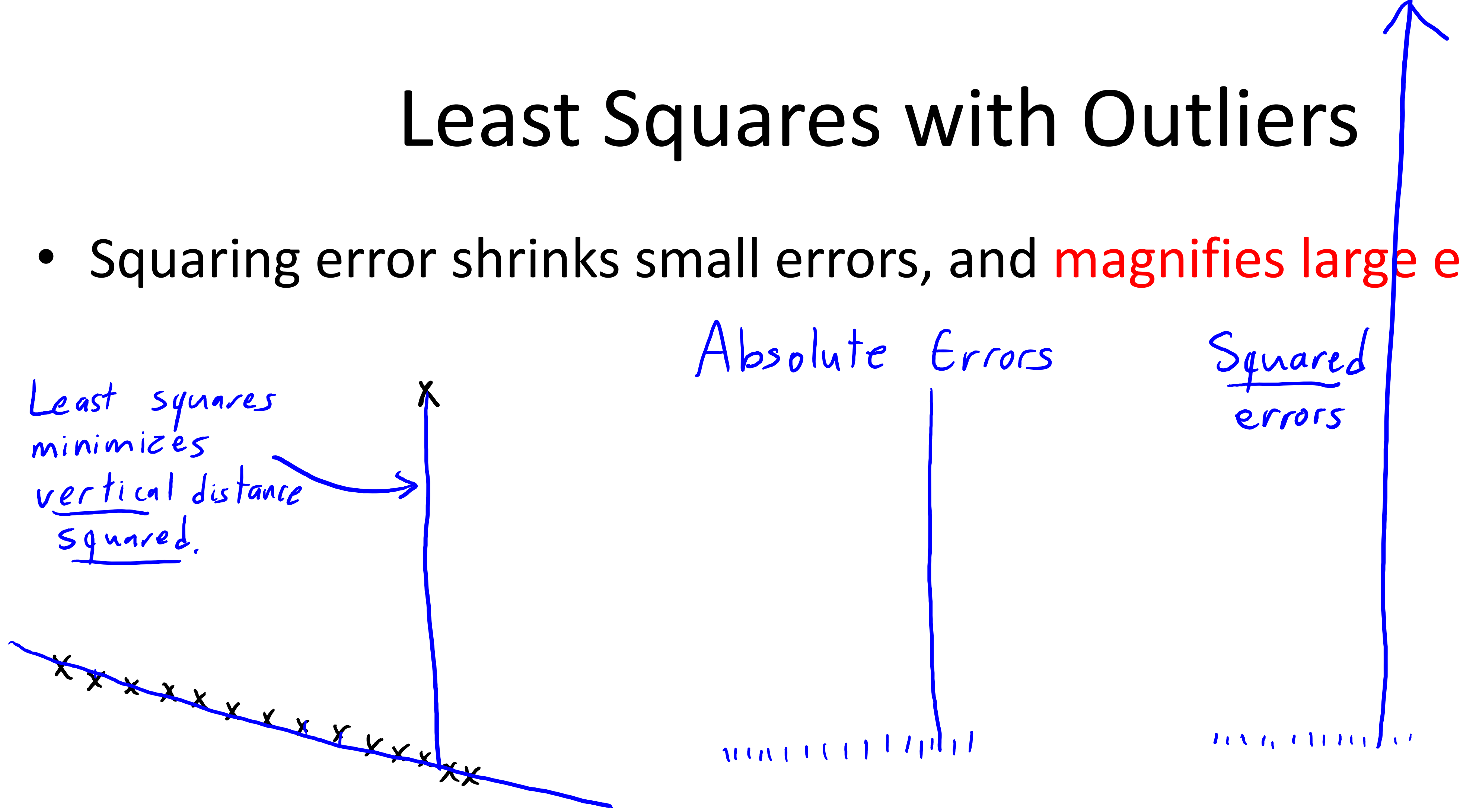
- Consider least squares problem with outliers in 'y':


"outlier" that doesn't follow trend
This is what least squares will actually do.

- Least squares is very sensitive to outliers.

# Least Squares with Outliers

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

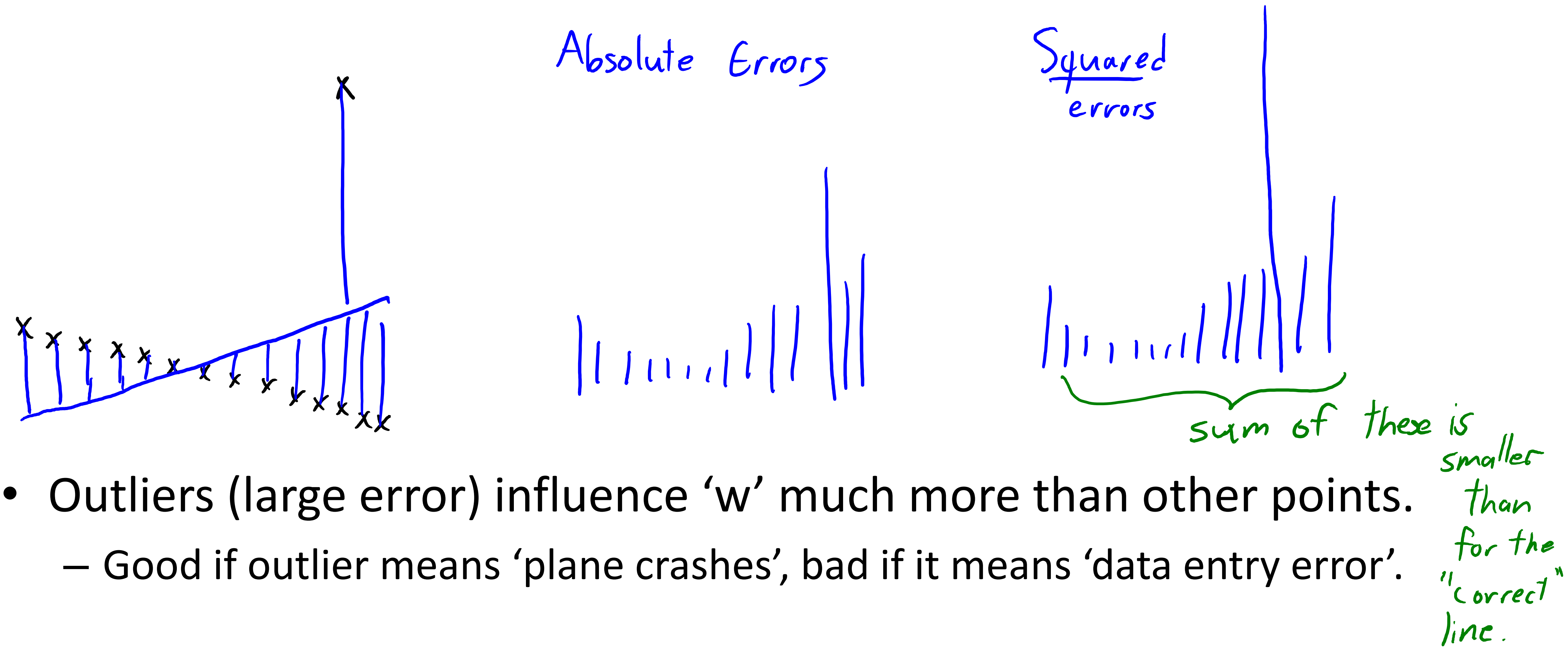


- Outliers (large error) influence 'w' much more than other points.

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'.

# 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:

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

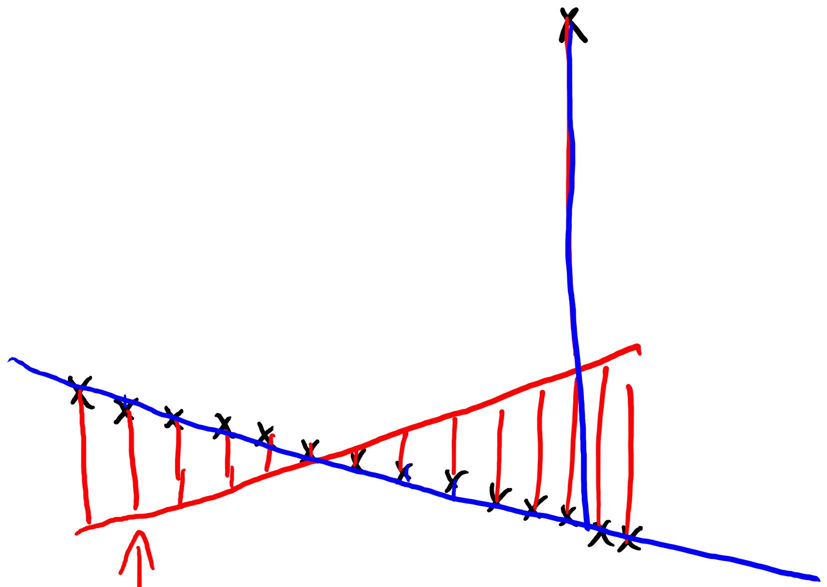
Least absolute error:

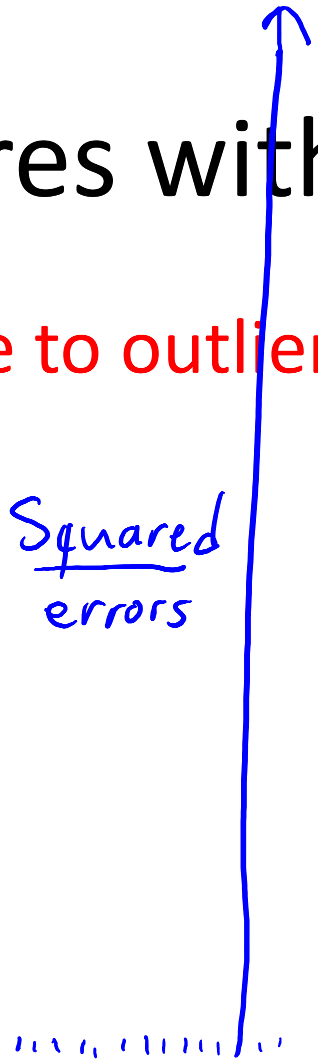
$$f(w) = \|Xw - y\|_1$$

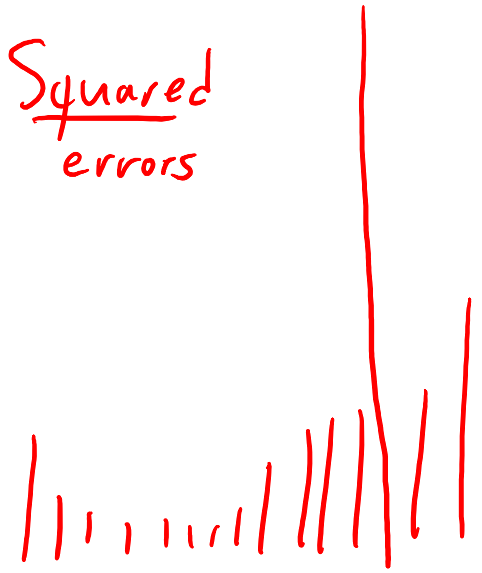
$$\sum_{i=1}^{n} |w^T x_i - y_i| = \sum_{i=1}^{n} |r_i| = \|r\|_1 = \|Xw - y\|_1$$

# Least Squares with Outliers

- Least squares is very sensitive to outliers.



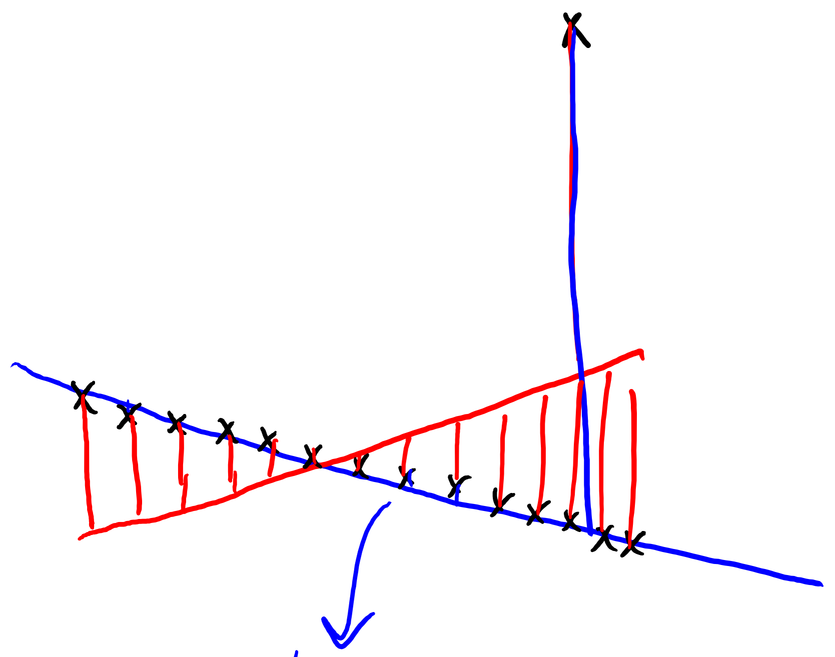


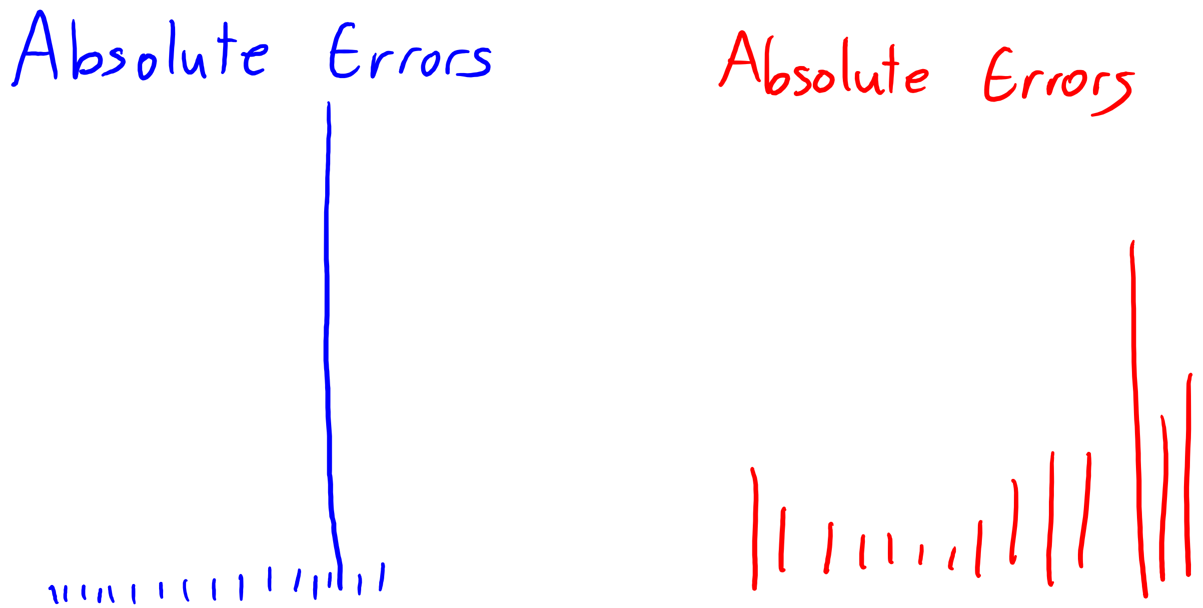


Linear model 'w' minimizing $f(w) = \frac{1}{2}\|Xw - y\|^2$

# Least Squares with Outliers

- Absolute error is more robust to outliers:

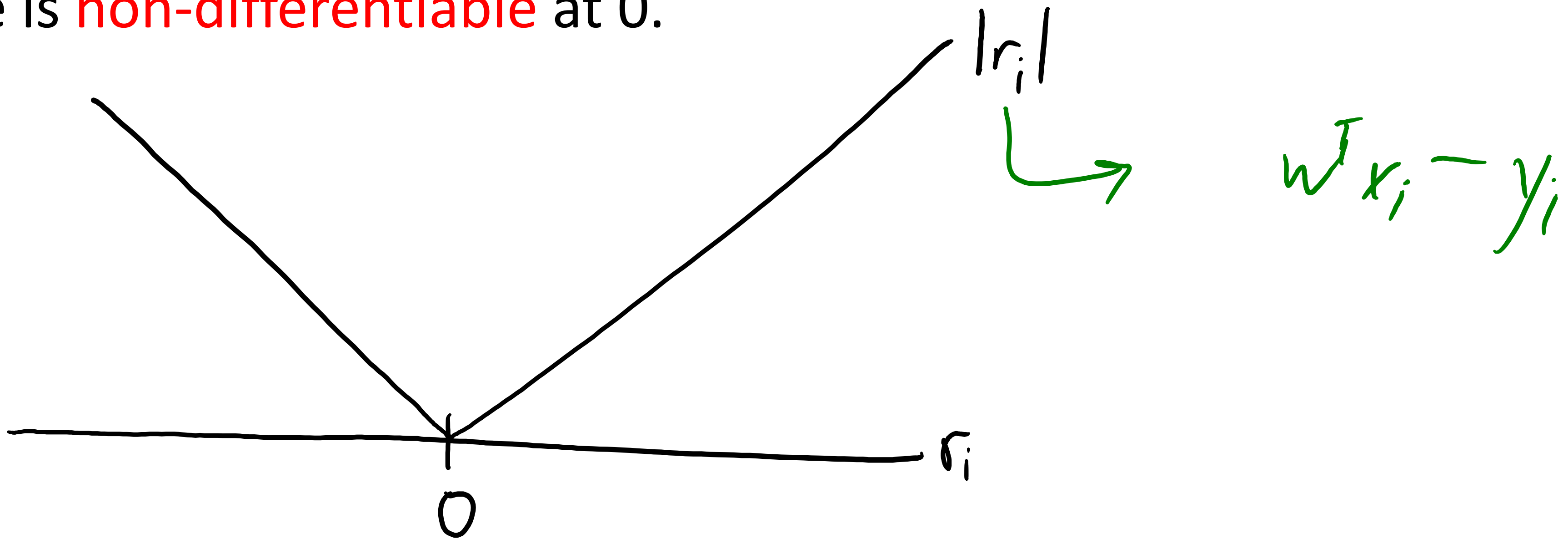




Linear model 'w' minimizing $f(w) = \|Xw - y\|_1 = \sum_{i=1}^{n} |w^T x_i - y_i|$

# 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.



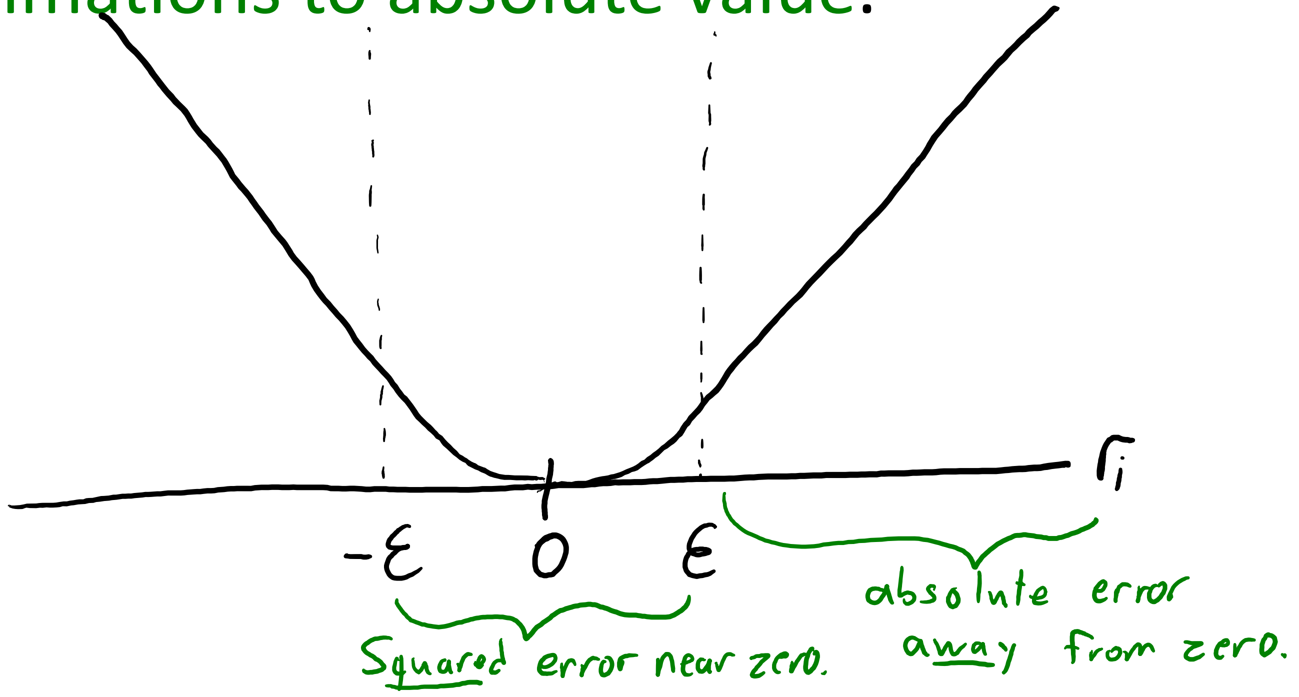
  - Generally, harder to minimize non-smooth than smooth functions.
    - Unlike smooth functions, the gradient may not get smaller near a minimizer.
  - To apply gradient descent, we'll use a smooth approximation.

# Smooth Approximations to the L1-Norm

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

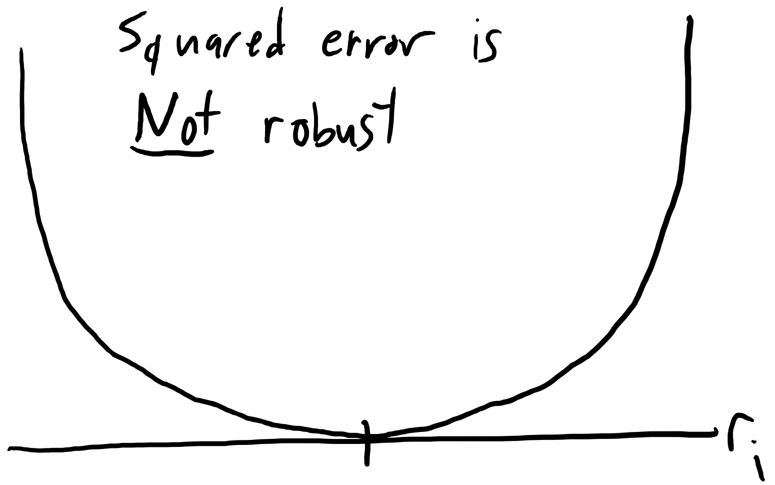
$$f(w) = \sum_{i=1}^{n} h(w^T x_i - y_i)$$

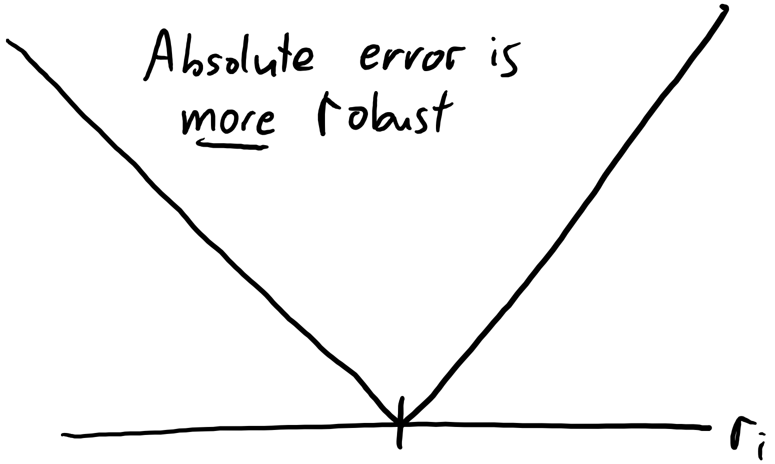
$$h(r_i) = \begin{cases} \frac{1}{2} r_i^2 & \text{for } |r_i| \leq \varepsilon \\ \varepsilon(|r_i| - \frac{1}{2}\varepsilon) & \text{otherwise} \end{cases}$$

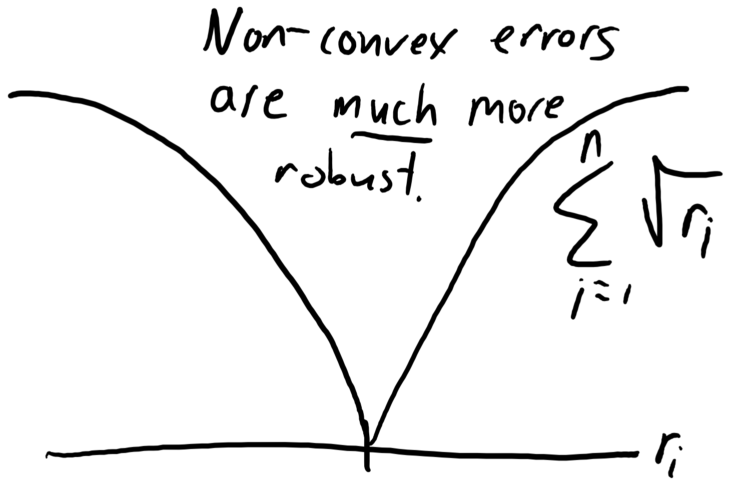


  - Note that 'h' is differentiable: h'(ε) = ε and h'(-ε) = -ε.
  - This 'f' is convex but setting $\nabla f(x) = 0$ does not give a linear system.
    - But we can minimize the Huber loss using gradient descent.

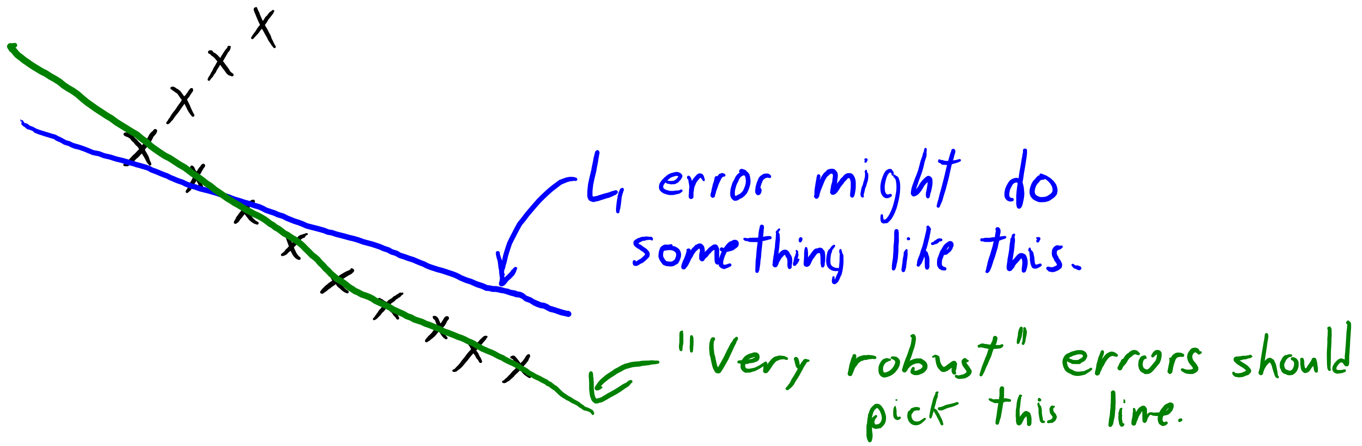
# Very Robust Regression



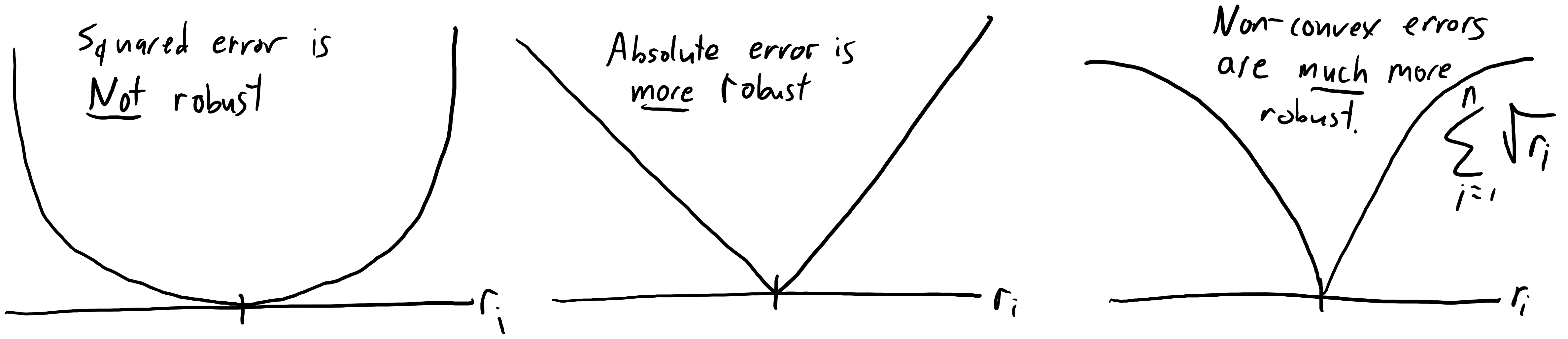




- Non-convex errors can be very robust:
  - Not influenced by outlier groups.

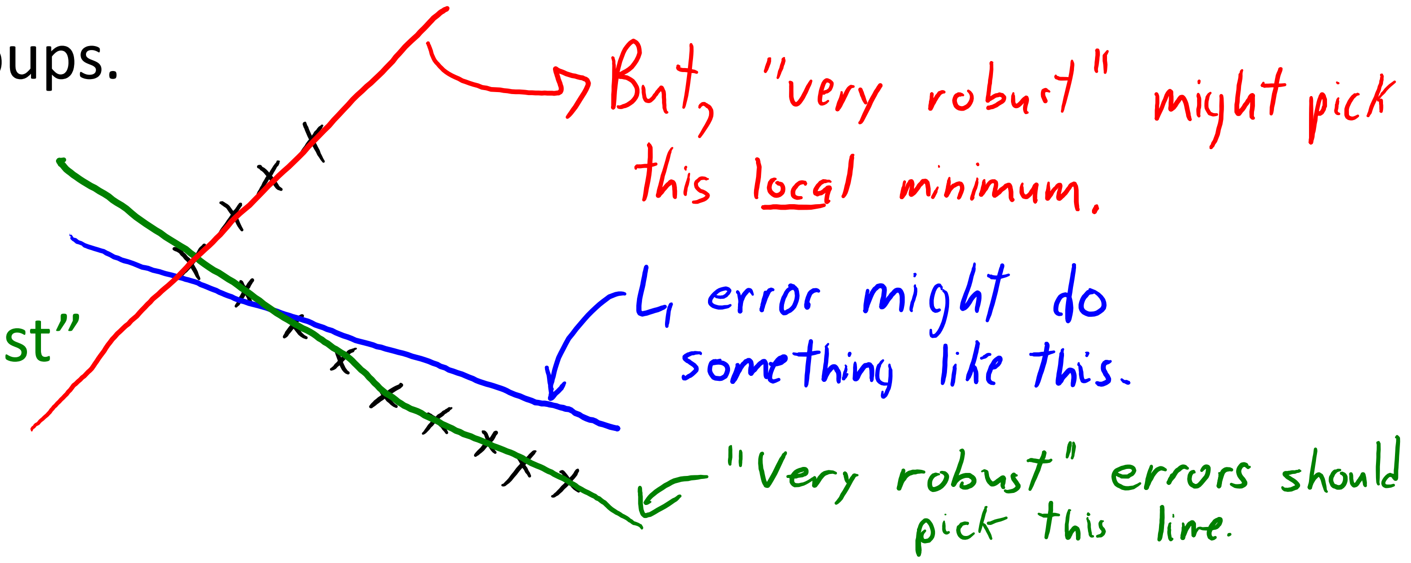


# Very Robust Regression



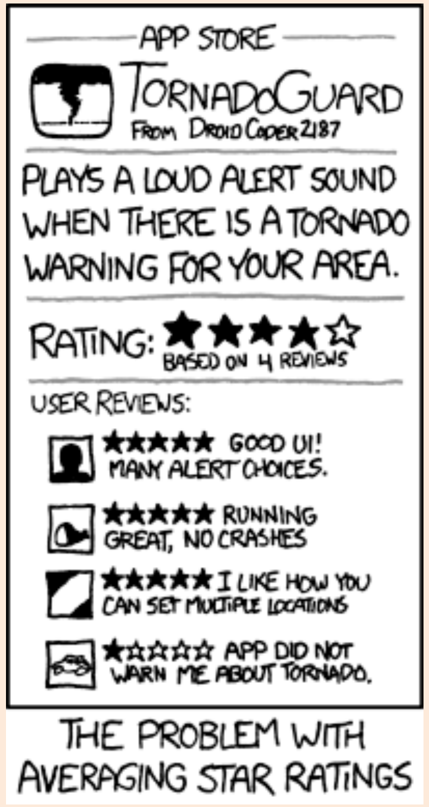
Squared error is Not robust
$r_i$
Absolute error is more robust
$r_i$
Non-convex errors are much more robust.
$\sum_{i=1}^{n} \sqrt{r_i}$
$r_i$

- 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.



But, "very robust" might pick this local minimum.
$L_1$ error might do something like this.
"Very robust" errors should pick this line.

# Motivation for Modeling Outliers

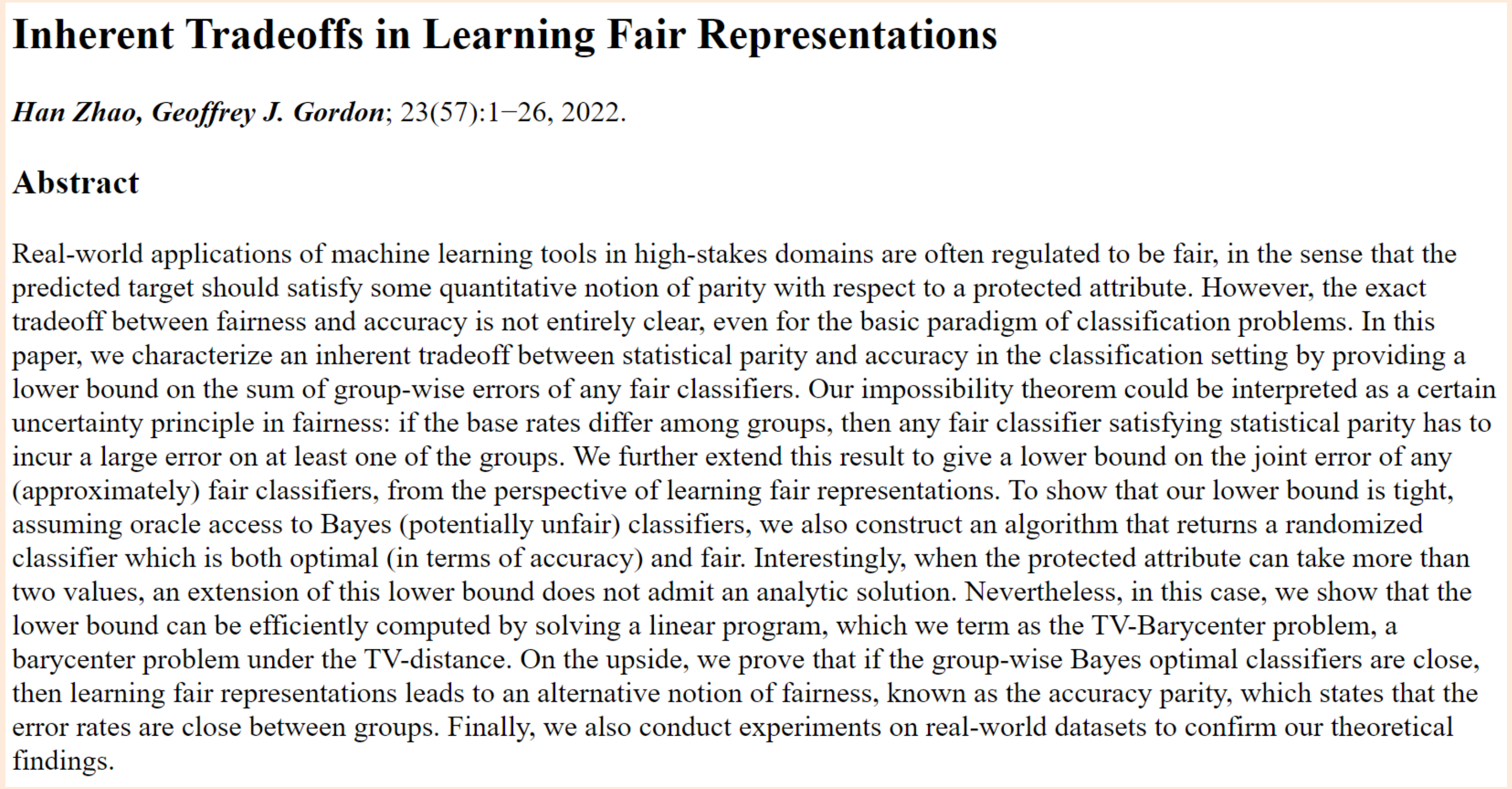

APP STORE
TORNADOGUARD
FROM DROIDCODER2187
PLAYS A LOUD ALERT SOUND WHEN THERE IS A TORNADO WARNING FOR YOUR AREA.
RATING: ★★★★☆ BASED ON 4 REVIEWS
USER REVIEWS:
★★★★★ GOOD UI! MANY ALERT CHOICES.
★★★★★ RUNNING GREAT, NO CRASHES
★★★★★ I LIKE HOW YOU CAN SET MULTIPLE LOCATIONS
★☆☆☆☆ APP DID NOT WARN ME ABOUT TORNADO.
THE PROBLEM WITH AVERAGING STAR RATINGS

- 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?

https://xkcd.com/937/

## Accuracy vs. Fairness Trade-Off?

- Improving test error might need to make fairness worse?
  - If you chase you outliers you might worsen generalization.
  - If you do not chase the outliers you might worsen fairness.
- Recent related paper:



**Inherent Tradeoffs in Learning Fair Representations**

***Han Zhao, Geoffrey J. Gordon***; 23(57):1−26, 2022.

**Abstract**

Real-world applications of machine learning tools in high-stakes domains are often regulated to be fair, in the sense that the predicted target should satisfy some quantitative notion of parity with respect to a protected attribute. However, the exact tradeoff between fairness and accuracy is not entirely clear, even for the basic paradigm of classification problems. In this paper, we characterize an inherent tradeoff between statistical parity and accuracy in the classification setting by providing a lower bound on the sum of group-wise errors of any fair classifiers. Our impossibility theorem could be interpreted as a certain uncertainty principle in fairness: if the base rates differ among groups, then any fair classifier satisfying statistical parity has to incur a large error on at least one of the groups. We further extend this result to give a lower bound on the joint error of any (approximately) fair classifiers, from the perspective of learning fair representations. To show that our lower bound is tight, assuming oracle access to Bayes (potentially unfair) classifiers, we also construct an algorithm that returns a randomized classifier which is both optimal (in terms of accuracy) and fair. Interestingly, when the protected attribute can take more than two values, an extension of this lower bound does not admit an analytic solution. Nevertheless, in this case, we show that the lower bound can be efficiently computed by solving a linear program, which we term as the TV-Barycenter problem, a barycenter problem under the TV-distance. On the upside, we prove that if the group-wise Bayes optimal classifiers are close, then learning fair representations leads to an alternative notion of fairness, known as the accuracy parity, which states that the error rates are close between groups. Finally, we also conduct experiments on real-world datasets to confirm our theoretical findings.

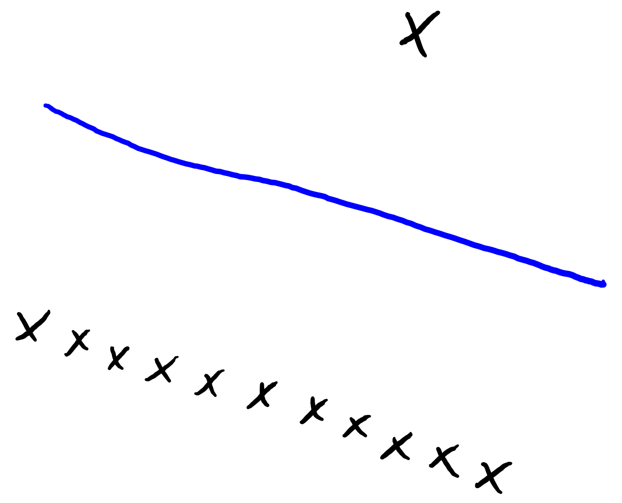
https://www.jmlr.org/papers/v23/21-1427.html

# "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 or you perform badly on a group.
- In this case you could use something like the infinity-norm:

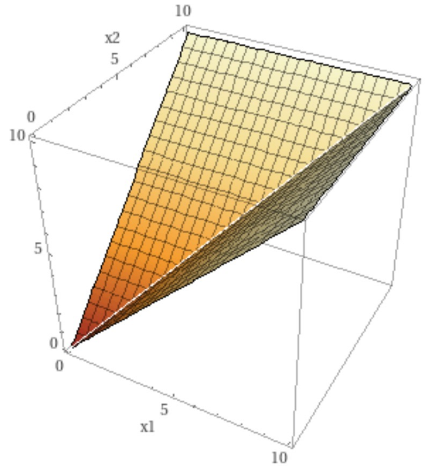
$$f(w) = \|Xw - y\|_\infty$$

where $\|r\|_\infty = \max_i \{|r_i|\}$



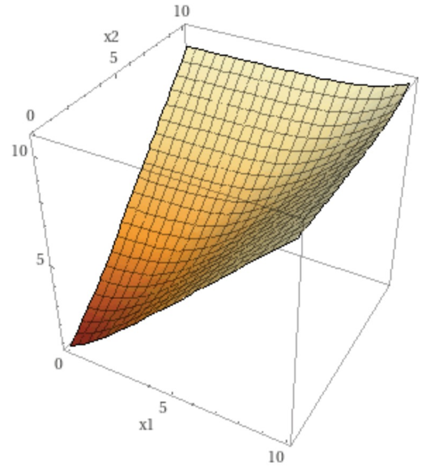
- Very sensitive to outliers ("brittle"), but minimizes highest error.
  - Different than previous errors, which were all some sort of average.

# Log-Sum-Exp Function



- As with the $L_1$-norm, the $L_\infty$-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 will 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:

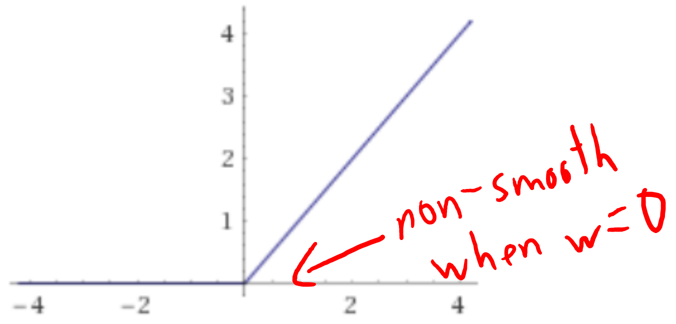
$$\max_i\{z_i\} \approx \log\left(\sum_i \exp(z_i)\right)$$

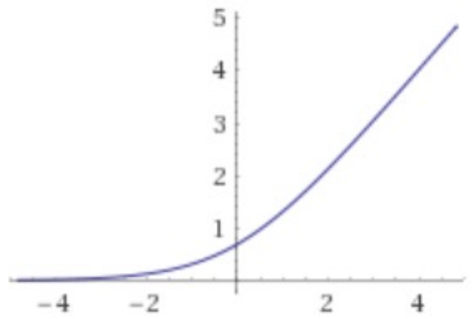
- If there aren't "close" values, it's really close to the max.

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)):



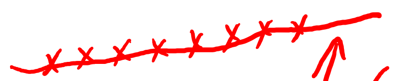


# Part 3 Key Ideas: Linear Models, Least Squares

- 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 <u>exactly</u> 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 ($L_\infty$) error is more sensitive to outliers.
- $L_1$ and $L_\infty$ 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.
  - $L_\infty$ 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.

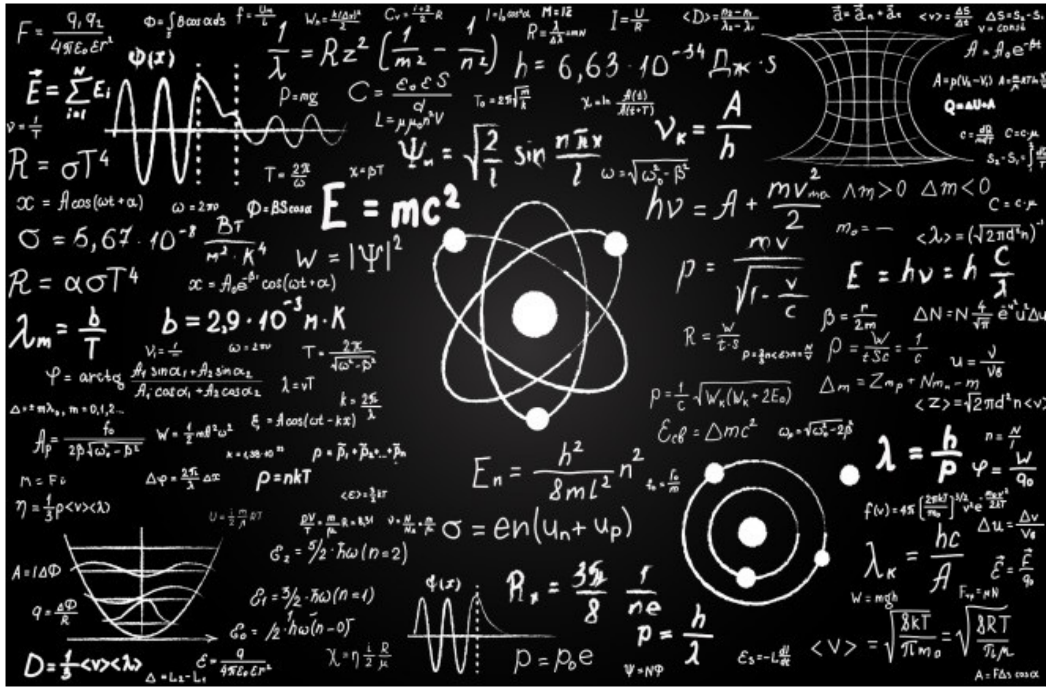
(we are not done Part 3, but nothing after this point will be tested on the midterm)

## Finding the "True" Model

- To measure performance we have focused on minimize test error.
  - This is good if our goal is to predict well on new IID data
  - But this is a weird way to do science!
    - "It's true there's been a lot of work on trying to apply statistical models to various linguistic problems. I think there have been some successes, but a lot of failures. There is a notion of success ... which I think is novel in the history of science. It interprets success as approximating unanalyzed data." Noam Chomsky.

# Finding the “True” Model

- To measure performance we have focused on minimize test error.
  - This is good if our goal is to predict well on new IID data
  - But this is a weird way to do science!
- We normally want to design simple models that explain the world.
  - Might work even if new data is not IID!

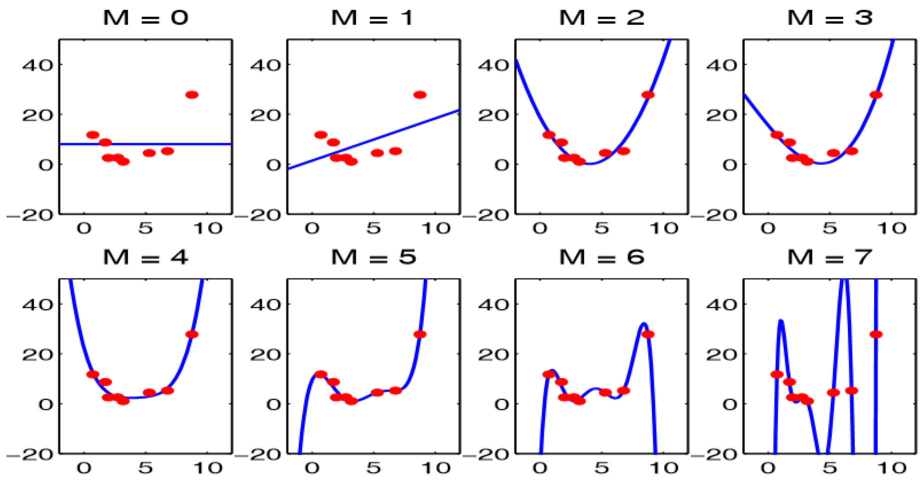


  - Next topic: finding the “true” model.
    - Hint: it is hard unless things are simple!

https://www.discovermagazine.com/the-sciences/the-5-most-important-scientific-equations-of-all-time

# Finding the "True" Model

- Consider a simple case of trying to 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 too large.
    (training error always decreases as you increase 'p')

# Finding the "True" Model

- Consider a simple case of trying to 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 (due to optimization bias).

  - Consider a case where the true model has p=2 (quadratic function).
    - We fit a quadratic function $y_i = 2x_i^2 – 5$, and a cubic function $y_i = 0.00001x_i^3 + 2x_i^2 - 5$.
    - Cubic is wrong, but by chance might get a lower error on a particular validation set.
      - If we try many models, there are more "chances" to randomly get a lower validation error.

# 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.

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

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 λ > 0 controls how strong we penalize complexity.
    - "You need to decrease the training error by least λ to increase 'k' by 1".

- Using (λ = 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.

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

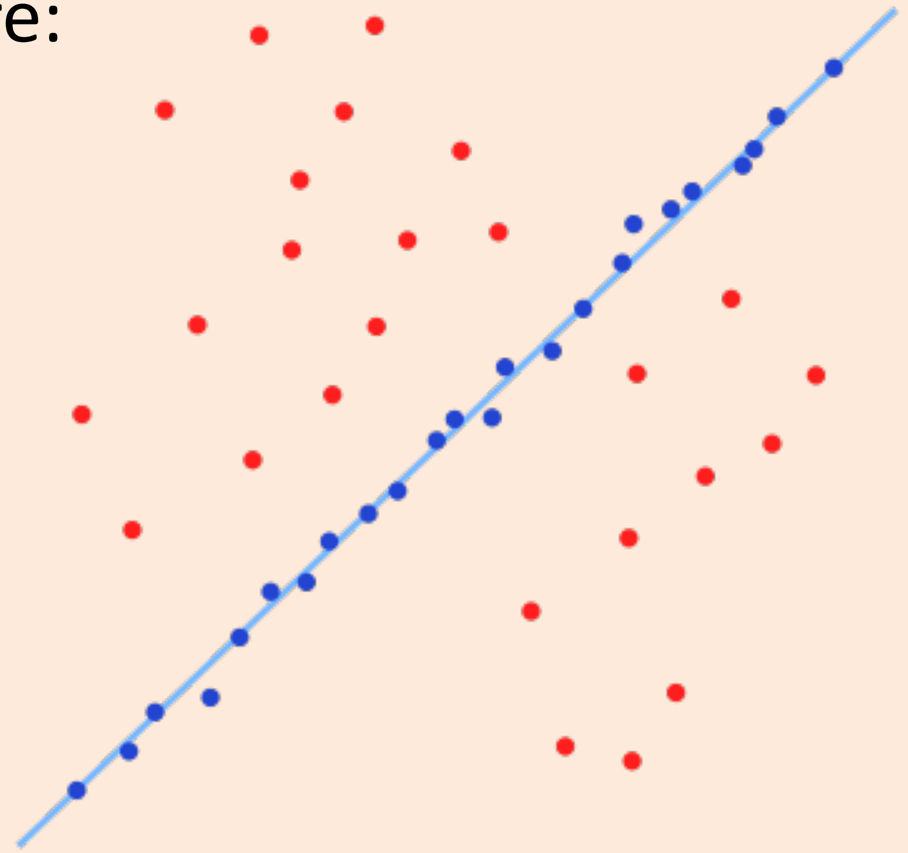
## Summary

- 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?

# Random Sample Consensus (RANSAC)

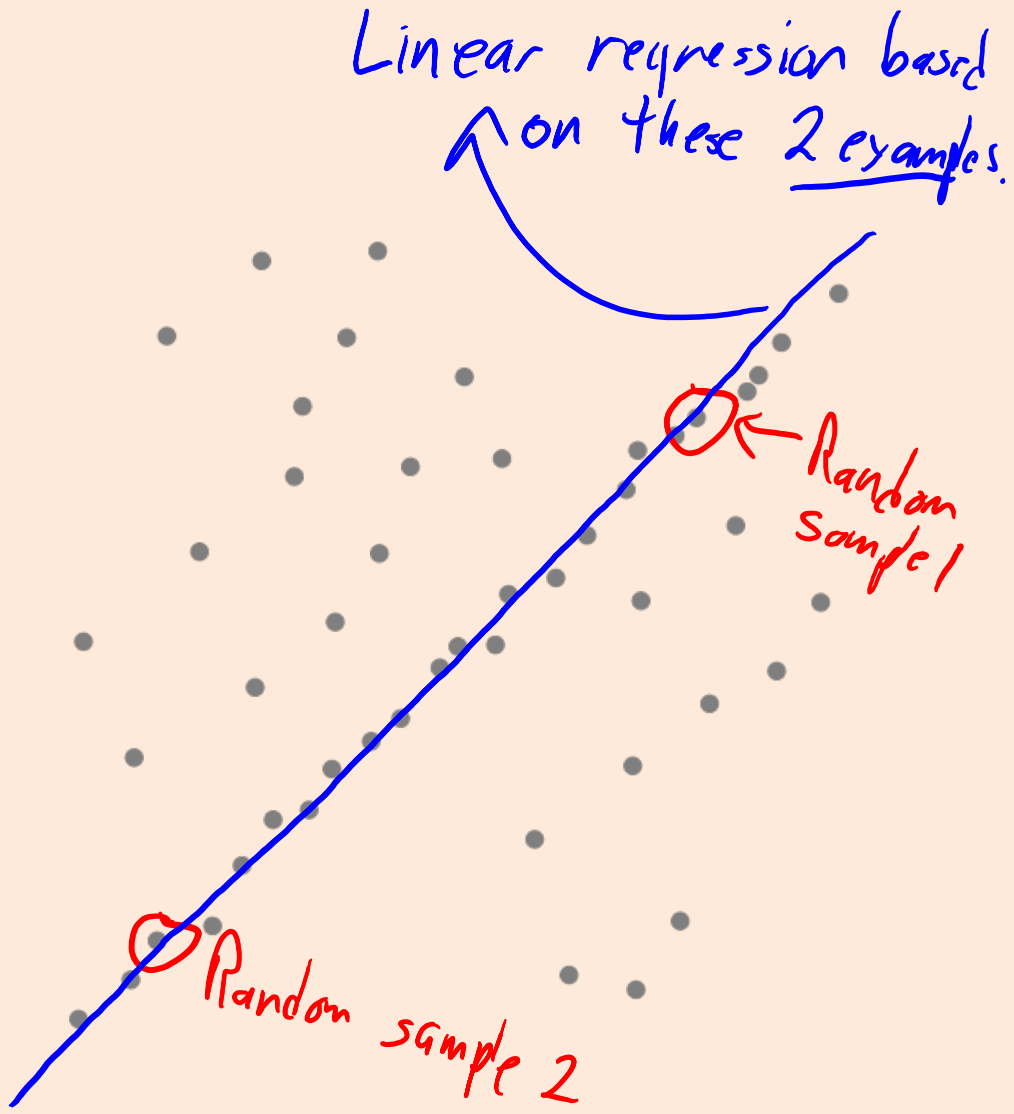
- In computer vision, a widely-used generic framework for robust fitting is random sample consensus (RANSAC).
- This is designed for the scenario where:
  - You have a large number of outliers.
  - Majority of points are "inliers": it's really easy to get low error on them.



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 $\beta = \max_i \{z_i\}$

$$\log\left(\sum_i \exp(z_i)\right) = \log\left(\sum_i \exp(z_i - \beta + \beta)\right)$$

$$= \log\left(\sum_i \exp(z_i - \beta)\exp(\beta)\right)$$

$$= \log\left(\exp(\beta)\sum_i \exp(z_i - \beta)\right)$$

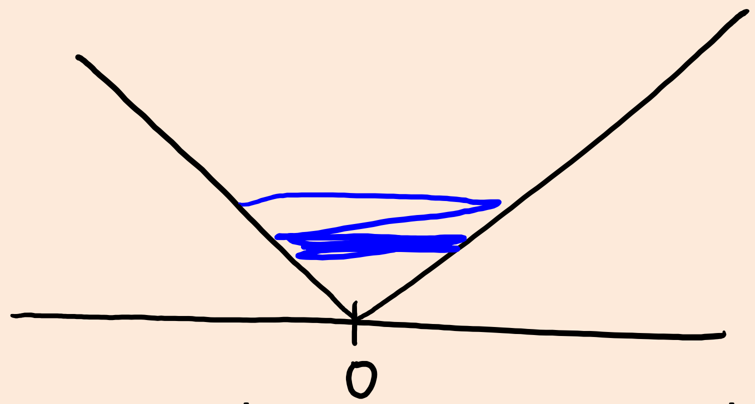
$$= \log(\exp(\beta)) + \log\left(\sum_i \exp(z_i - \beta)\right)$$

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

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.

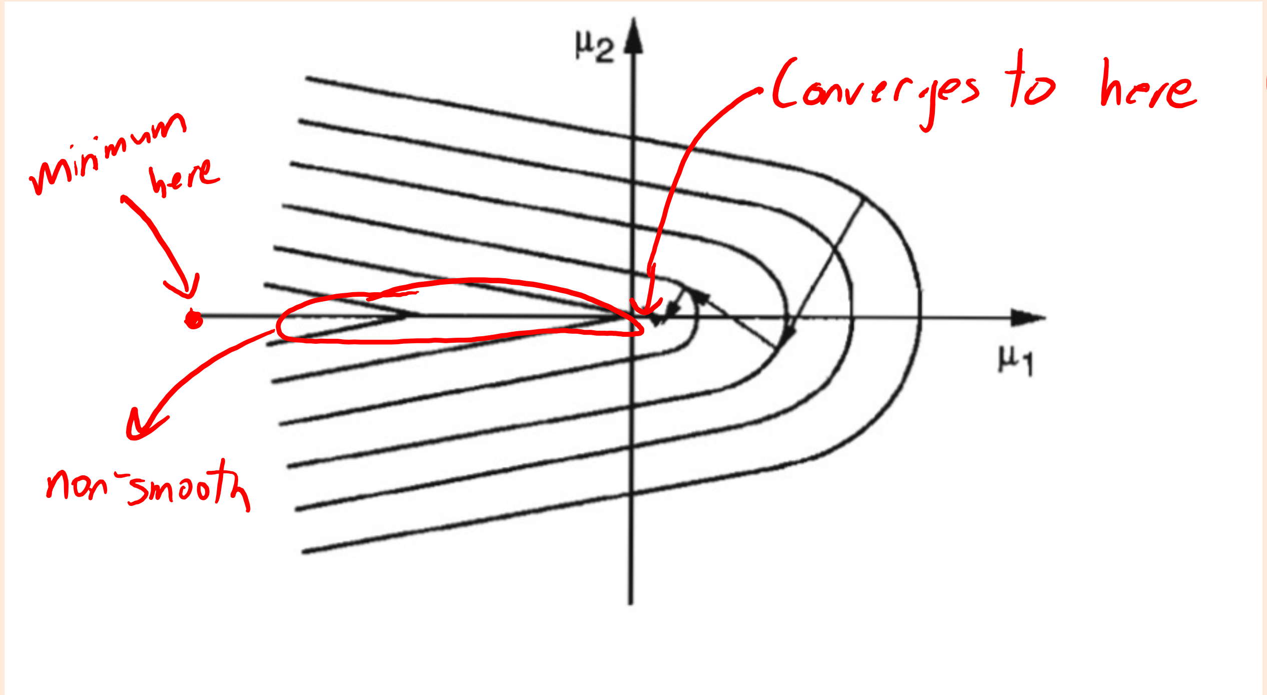


**Figure 6.3.8.** Contours and steepest ascent path for the function of Exercise 6.3.8.

(even though function is convex)

# 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 $\geq 0$.
  - 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 $\geq 0$)

So it's convex