DSC 140A Probabilistic Modeling & Machine Kearning

Lecture 5 | Part 1

Introduction

Empirical Risk Minimization (ERM)

- Step 1: choose a hypothesis class
 - We've chosen linear predictors.
- Step 2: choose a loss function
- Step 3: find H minimizing empirical risk
 - In case of linear predictors, equivalent to finding \vec{w} .

Minimizing Empirical Risk

► We want to minimize the **empirical risk**:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \ell(\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i)$$

Minimizing Empirical Risk

- For some losses there's a formula for the best \vec{w} .
 - **Example:** square loss.
 - But it might be too costly to use!
- For others, there isn't.
 - **Example:** absolute loss, Huber loss.
- In either case, we might use gradient descent.

Last Time

We addressed two issues with gradient descent.

- 1. Can be **expensive** to compute the exact gradient.
 - Especially when we have a large data set.
 - ► Solution: stochastic gradient descent.
- 2. Doesn't work as-is if risk is **not differentiable**.
 - Such as with the absolute loss.
 - Solution: subgradient descent.

Today

- Answer two outstanding questions:
- 1. How do we minimize the risk with respect to the **absolute loss**?
- 2. When is gradient descent **guaranteed** to work?

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Lecture 5 | Part 2

Minimizing Risk w.r.t. Absolute Loss

Regression with Absolute Loss

► The risk with respect to the absolute loss:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|$$

- We were stuck before.
 - ► This risk is **not differentiable**.

Now: we can minimize the risk with respect to the absolute loss using subgradient descent.

Subgradient Descent

To minimize $f(\vec{z})$:

- Pick arbitrary starting point $\vec{z}^{(0)}$, a decreasing learning rate schedule $\eta(t) > 0$.
- Until convergence, repeat:
 - **Compute a subgradient** \vec{s} of f at $\vec{z}^{(i)}$.
 - ► Update $\vec{z}^{(t+1)} = \vec{z}^{(t)} \eta(t) \vec{s}$
- ▶ When converged, return $\vec{z}^{(t)}$.

Subgradient of Empirical Risk

- We need a **subgradient** of the empirical risk with respect to the absolute loss.
- ► **Useful fact**: the subgradient of a sum is the sum of the subgradients.¹
- So it suffices to find a subgradient of the loss function:

subgrad
$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \text{subgrad } \ell(\vec{w}; \vec{x}^{(i)}, y_i)$$

¹At least, for convex functions.

We need a subgradient of the absolute loss.

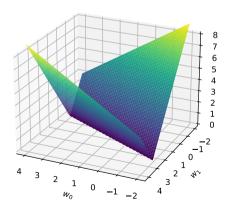
$$\ell_{abs}(\vec{w} \cdot Aug(\vec{x}^{(i)}), y_i) = |\vec{w} \cdot Aug(\vec{x}^{(i)}) - y_i|$$

An equivalent piecewise definition:

$$\ell_{\mathsf{abs}}(\vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}), y_i) = \begin{cases} \vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}) - y_i, & \text{if } \vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}) > y_i, \\ y_i - \vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}) < y_i, \\ 0, & \text{if } \vec{w} \cdot \mathsf{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

The Absolute Loss

- Gradient exists except at $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i$.
 - Here, we need a subgradient.



$$\frac{d}{d\vec{w}} \left(\vec{w} \cdot A w (\vec{x}^{(c)}) - y_{i} \right) = A w (\vec{x}^{(c)})$$

Exercise

What is the gradient when $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i$? What about when $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i$?

$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = \begin{cases} \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ y_i - \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ 0, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

$$\ell_{abs}(\vec{w} \cdot Aug(\vec{x}^{(i)}), y_i) = |\vec{w} \cdot Aug(\vec{x}^{(i)}) - y_i|$$

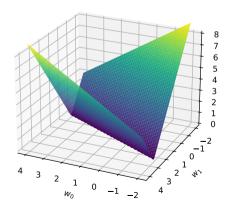
If
$$\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i$$
:

- Loss is $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) y_i$.
- ► Gradient is Aug($\vec{x}^{(i)}$).

If
$$\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i$$
:

- ► Loss is $y_i \vec{w} \cdot \text{Aug}(\vec{x}^{(i)})$.
- ► Gradient is Aug($\vec{x}^{(i)}$).

The zero vector works as a subgradient.



Our subgradient of the absolute loss:

$$s(\vec{w}; \vec{x}^{(i)}, y_i) = \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

Minimizing the Absolute Loss

► The subgradient of the empirical risk is the average of the subgradients of the loss:

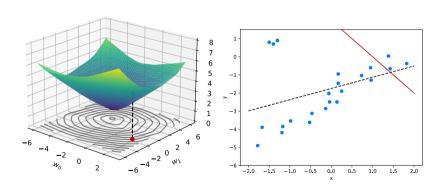
subgrad. of
$$R(\vec{w})$$

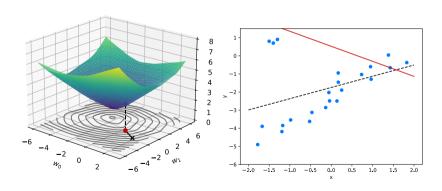
= $\frac{1}{n} \sum_{i=1}^{n} s(\vec{w}, \vec{x}^{(i)}, y_i)$
= $\frac{1}{n} \sum_{i=1}^{n} \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$

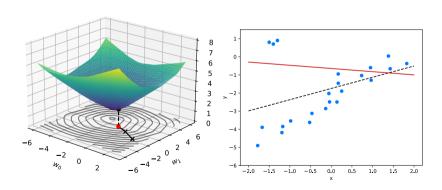
Subgradient Descent

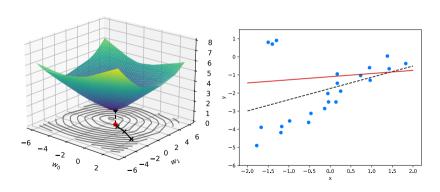
- We minimize the empirical risk with respect to the absolute loss using subgradient descent.
- Pick an initial $\vec{w}^{(0)}$, a decreasing learning rate schedule $\eta(t) > 0$.
- Until convergence, repeat:
 - Update

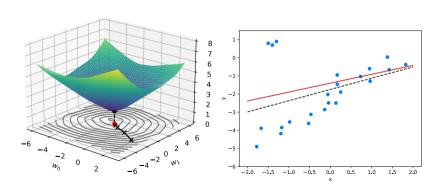
$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta(t) \times \frac{1}{n} \sum_{i=1}^{n} \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

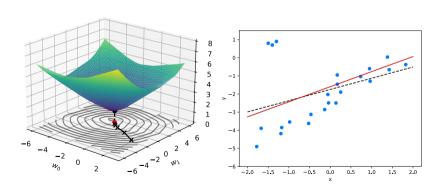


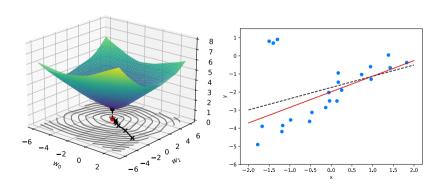


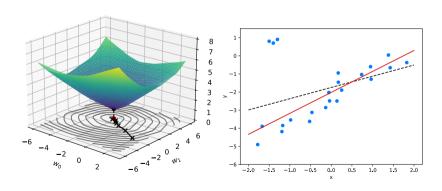












In Practice

We've minimized the risk with respect to the absolute loss.

- This approach has different names:
 - Quantile regression, median regression
 - Minimum Absolute Deviations (MAD)

Solvable by (S)GD, or as a linear program.

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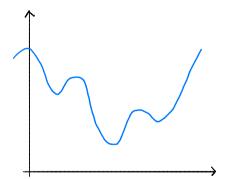
Lecture 5 | Part 3

Convexity

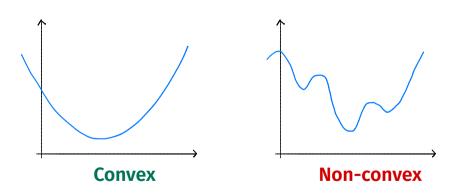
Question

► When is gradient descent guaranteed to work?

Not here...

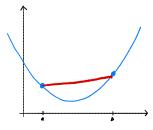


Convex Functions



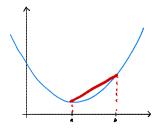
► f is convex if for every a, b the line segment between

$$(a, f(a))$$
 and $(b, f(b))$



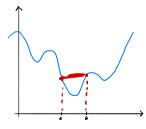
► f is convex if for every a, b the line segment between

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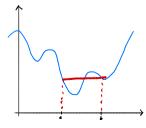
► f is convex if for every a, b the line segment between

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 and $(b, f(b))$



► f is convex if for every a, b the line segment between

$$(a, f(a))$$
 and $(b, f(b))$



Other Terms

- ► If a function is not convex, it is **non-convex**.
- Strictly convex: the line lies strictly above curve.
- Concave: the line lines on or below curve.

Exercise

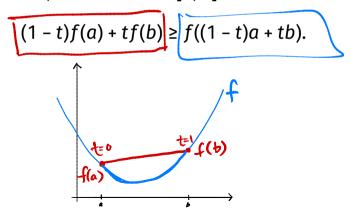
True or **False**: a convex function must have a unique global minimum.

True or **False**: a local minimum of a convex function is always a global minimum.

True or **False**: a *strictly* convex function must have a unique global minimum.

Convexity: Formal Definition $f(\frac{1}{2},\frac{1}{2},\frac{1}{2}) = f(\frac{1}{2},\frac{1}{2})$

▶ A function $f : \mathbb{R} \to \mathbb{R}$ is **convex** if for every choice of $a, b \in \mathbb{R}$ and $t \in [0, 1]$:

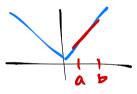


Exercise

Using the definition, is f(x) = |x| convex?

There one three cases

Core 1:
$$a \in b$$
 are positive
 $(1-t)f(a) + tf(b) = (1-t)|a| + t|b|$
 $= (1-t)a + tb$
 $= (1-t)a + tb|$
 $= f(1-t)a + tb|$



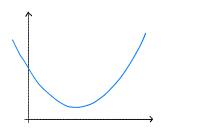
Case 2 & 3:

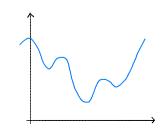
Another View: Second Derivatives

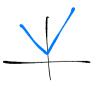
► If $\frac{d^2f}{dx^2}(x) \ge 0$ for all x, then f is convex.

Example:
$$f(x) = x^4$$
 is convex. $f''(x) = 1/2x^2 \ge 0$

► Warning! Only works if f is twice differentiable!







Another View: Second Derivatives

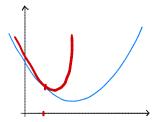
- ► "Best" straight line at x_0 :
 - $f_1(x) = f(x_0) + f'(x_0) \cdot (x x_0)$

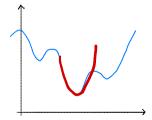
$$\triangleright$$
 "Best" parabola at x_0 :

- $f_2(x) = f(x_0) + f'(x_0) \cdot (x x_0) + \frac{1}{2}f''(x_0) \cdot (x x_0)^2$
- Possibilities: upward-facing, downward-facing, flat.

Convexity and Parabolas

- Convex if for **every** x_0 , parabola is upward-facing (or flat).
 - ► That is, $f''(x_0) \ge 0$.

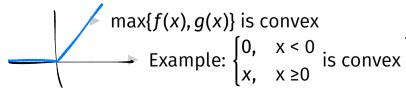




Proving Convexity Using Properties

Suppose that f(x) and g(x) are convex. Then:

- $w_1 f(x) + w_2 g(x)$ is convex, provided $w_1, w_2 \ge 0$
 - Example: $3x^2 + |x|$ is convex
- ightharpoonup g(f(x)) is convex, provided g is non-decreasing.
 - Example: e^{x^2} is convex



Note!

- ► These properties are useful for proving convexity for functions of **one variable**.
- Some of them will not generalize to higher dimensions.

Convexity and Gradient Descent

- Convex functions are (relatively) easy to optimize.
- Theorem: if f(x) is convex and "not too steep"² then (stochastic) (sub)gradient descent converges to a **global optimum** of f provided that the step size is small enough³

²Technically, c-Lipschitz

³step size related to steepness, should decrease like $1/\sqrt{\text{step }\#}$.

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Lecture 5 | Part 4

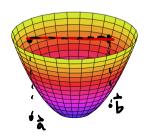
Convexity in Many Dimensions

Convexity: Definition

• $f(\vec{x})$ is **convex** if for **every** \vec{a} , \vec{b} the line segment between

$$(\vec{a}, f(\vec{a}))$$
 and $(\vec{b}, f(\vec{b}))$

does not go below the plot of f.



Convexity: Formal Definition

A function $f: \mathbb{R}^d \to \mathbb{R}$ is **convex** if for every choice of $\vec{a}, \vec{b} \in \mathbb{R}^d$ and $t \in [0, 1]$:

$$(1-t)f(\vec{a}) + tf(\vec{b}) \ge f((1-t)\vec{a} + t\vec{b}).$$

The Second Derivative Test

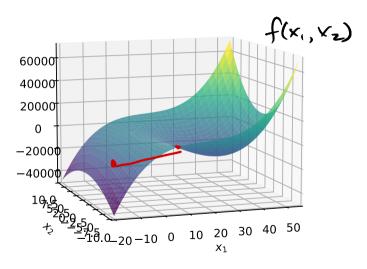
- ► For 1-dimensions functions:
 - convex if second derivative > 0.
- For d-dimensional functions: $f(x_1, x_2, ..., x_n)$
 - convex if ???

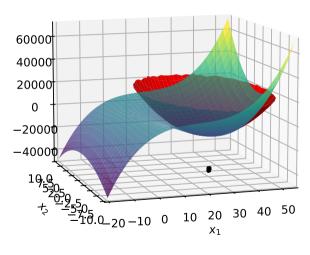
Second Derivatives in *d***-Dimensions**

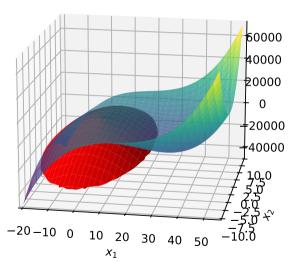
▶ In 2-dimensions, there are 4 second derivatives:

$$\triangleright \frac{\partial f^2}{\partial x_1^2}, \frac{\partial f^2}{\partial x_2^2}, \frac{\partial f^2}{\partial x_1 x_2}, \frac{\partial f^2}{\partial x_2 x_1}$$

- ▶ In *d*-dimensions, there are d^2 :
- The second derivatives describe the curvature of a paraboloid approximating f.







The Hessian Matrix

Create the Hessian matrix of second derivatives:

▶ For
$$f: \mathbb{R}^2 \to \mathbb{R}$$
:

$$H(\vec{x}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2} (\vec{x}) & \frac{\partial f^2}{\partial x_1 x_2} (\vec{x}) \\ \frac{\partial f^2}{\partial x_2 x_1} (\vec{x}) & \frac{\partial f^2}{\partial x_2^2} (\vec{x}) \end{pmatrix}$$

In General

▶ If $f: \mathbb{R}^d \to \mathbb{R}$, the **Hessian** at \vec{x} is:

$$H(\vec{x}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2} (\vec{x}) & \frac{\partial f^2}{\partial x_1 x_2} (\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_1 x_d} (\vec{x}) \\ \frac{\partial f^2}{\partial x_2 x_1} (\vec{x}) & \frac{\partial f^2}{\partial x_2^2} (\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_2 x_d} (\vec{x}) \\ \cdots & \cdots & \cdots \\ \frac{\partial f^2}{\partial x_d x_1} (\vec{x}) & \frac{\partial f^2}{\partial x_d^2} (\vec{x}) & \cdots & \frac{\partial f^2}{\partial x_d^2} (\vec{x}) \end{pmatrix}$$

Second Derivative Test

A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if for any $\vec{x} \in \mathbb{R}^d$, all **eigenvalues** of the Hessian matrix $H(\vec{x})$ are ≥ 0 .

For This Class...

You will not need to compute eigenvalues "by hand"...

- Unless the matrix is diagonal.
 - In which case, the eigenvalues are the diagonal entries.

Example

► The eigenvalues of this matrix are 5, 2, and 1.

$$\begin{pmatrix}
5 & 0 & 0 \\
0 & 2 & 0 \\
0 & 0 & 1
\end{pmatrix}$$

Exercise

Is $f(x,y) = e^x + e^y + x^2 - y^2$ convex?

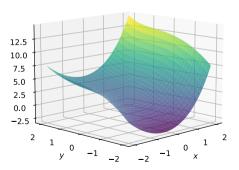
$$\frac{\partial f}{\partial x} = e^{x} + 2x \qquad \frac{\partial^{2} f}{\partial x^{2}} = e^{x} + 2$$

$$\frac{\partial f}{\partial y} = e^{y} - 2y \qquad \frac{\partial^{2} f}{\partial y^{2}} = e^{y} - 2 \qquad H(x,y) = \begin{pmatrix} e^{x} + 2 & 0 \\ 0 & e^{y} - 2 \end{pmatrix}$$

$$\frac{\partial^{2} f}{\partial x \partial y} = 0 \qquad H(0,0) = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix}$$

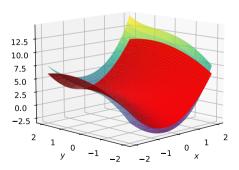
No

► The Hessian at (0,0) has a negative eigenvalue.



No

► The Hessian at (0,0) has a negative eigenvalue.



Exercise

Is $f(\vec{w}) = ||\vec{w}||^2$ convex?

$$||\vec{w}||^2 = |\vec{w}_1^2 + |\vec{w}_2^2 + \cdots + |\vec{w}_d^2|$$

$$|(\vec{w})|^2 = \begin{pmatrix} 2 & & \\ 0 & 2 & \\ & & \\ \end{pmatrix}$$

Note

► The second derivative test only works if *f* is twice differentiable.

A function can be convex without having a second derivative.

Properties

- We can often prove convexity using properties.
- Two useful properties:
 - Sums of convex functions are convex.
 - Affine compositions of convex functions are convex.

Sums of Convex Functions

Suppose that $f(\vec{x})$ and $g(\vec{x})$ are convex. Then $w_1 f(\vec{x}) + w_2 g(\vec{x})$ is convex, provided $w_1, w_2 \ge 0$.

Affine Composition

Suppose that $f(\vec{x})$ is convex. Let A be a matrix, and \vec{x} and \vec{b} be vectors. Then

$$g(\vec{x}) = f(A\vec{x} + \vec{b})$$

is convex as a function of \vec{x} .

Remember: a vector is a matrix with one column/row.

Useful!

Exercise

Consider the function

$$f(\vec{w}) = (\vec{x} \cdot \vec{w} - y)^2$$

Is this function convex as a function of \vec{w} ?

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Lecture 5 | Part 5

Convex Loss Functions

Empirical Risk Minimization (ERM)

- Step 1: choose a hypothesis class
 - We've chosen linear predictors, $H(\vec{x}) = \text{Aug}(\vec{x}) \cdot \vec{w}$.
- ► Step 2: choose a loss function
- ► Step 3: find w minimizing **empirical risk**
 - Some choices of loss function make this easier.

Convexity and Gradient Descent

- Convex functions are (relatively) easy to optimize.
- Theorem: if f(x) is convex and "not too steep"⁴ then (stochastic) (sub)gradient descent converges to a **global optimum** of f provided that the step size is small enough⁵.

⁴Technically, c-Lipschitz

⁵step size related to steepness, should decrease like $1/\sqrt{\text{step }\#}$

Convex Loss

- ▶ **Recall:** sums of convex functions are convex.
- ▶ **Implication:** if loss function is convex as a function of \vec{w} , so is the empirical risk, $R(\vec{w})$

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(\operatorname{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i)$$

Takeaway: Convex losses make ERM easier.

Example: Square Loss

Recall the square loss for a linear predictor:

$$\ell_{sq}(Aug(\vec{x}) \cdot \vec{w}, y) = (Aug(\vec{x}) \cdot \vec{w} - y)^2$$

- ► This is **convex** as a function of \vec{w} .
- Proof: a few slides ago.

Example: Absolute Loss

Recall the absolute loss for a linear predictor:

$$\ell_{abs}(Aug(\vec{x}) \cdot \vec{w}, y) = |Aug(\vec{x}) \cdot \vec{w} - y|$$

► This is **convex** as a function of \vec{w} .

Linear Predictors

- It's also important that we've chosen linear predictors.
- A loss that is **convex** in \vec{w} for linear $H_1(x)$ may be **non-convex** for non-linear $H_2(x)$.
- Example: square loss.
 - If $H_1(x) = W_0 + W_1 x$, then $(W_0 + W_1 x y)^2$ is **convex**.
 - ► If $H_2(x) = w_0 e^{w_1 x}$, then $(w_0 e^{w_1 x} y)^2$ is **non-convex**.

Summary

- By combining 1) linear predictors and 2) a convex loss function, we make ERM easier.
- Many machine learning algorithms are linear predictors with convex loss functions.
 - ► As we'll see...

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Lecture 5 | Part 6

From Theory to Practice

Gradient Descent

- We've spent three lectures on gradient descent.
- A powerful optimization algorithm.
- In practice, we use extensions of (stochastic) gradient descent.

Extensions of SGD

- Newton's method
 - Second order optimization, using the Hessian.
 - Can converge in fewer steps.
 - But the Hessian is expensive to compute.
- Adagrad, RMSprop, Adam
 - ► SGD with adaptive learning rates.
 - Used heavily in training of deep neural networks.

Non-Convex Optimization

- So far, we've only seen convex risks.
- But there's an important class of machine learning algorithms that have non-convex risks.
- Namely: deep neural networks.

Empirical Risk Minimization (ERM)

- Step 1: choose a hypothesis class
 - Deep neural networks.
- Step 2: choose a loss function
- ► Step 3: find w minimizing empirical risk

Deep Learning

- A deep neural network is a prediction function $H(\vec{x}; \vec{w})$ composed of many layers.
- Typically, H is not linear in \vec{w} .
- ► The risk becomes highly **non-convex**.
 - Even, for example, the square loss.
- How do we minimize the empirical risk?

Answer: SGD

- We use stochastic gradient descent (and extensions).
 - Even though the empirical risk is **non-convex**.
 - The optimization problem becomes much harder.
- SGD may not find a global minimum of the risk.
- But often finds a "good enough" local minimum.

Next Time

HOXE IIIII

► Linear classification.