# Gradient Descent and Loss Functions

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(Slides credit to David Rosenberg, He He, et al.)

NYU

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# Lecture Slides

- For those of you who want to take notes on your tablets.
- Otherwise, slides will be shared on the course website after the lecture.

# Homework 1

- Homework 1 will be released soon. You have until Oct 1 noon (12pm) to finish.
- Submit PDF and code to Gradescope.
- Course website: https://nyu-cs2565.github.io/2024-fall/

# Review: ERM

# Our Machine Learning Setup

## Prediction Function

A **prediction function** gets input $x$ and produces an output $\hat{y} = f(x)$.

## Loss Function

A **loss function** $\ell(\hat{y}, y)$ evaluates an action in the context of the outcome $y$.

# Risk and the Bayes Prediction Function

**Definition**

The **risk** of a prediction function $f : \mathcal{X} \to \mathcal{Y}$ is

$$R(f) = \mathbb{E}\ell(f(x), y).$$

In words, it's the **expected loss** of $f$ on a new example $(x, y)$ drawn randomly from $P_{\mathcal{X}\times\mathcal{Y}}$.

**Definition**

A **Bayes prediction function** $f^*$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* \in \arg\min_f R(f),$$

- The risk of a Bayes prediction function is called the **Bayes risk**.

# The Empirical Risk

Let $\mathcal{D}_n = ((x_1, y_1), \ldots, (x_n, y_n))$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X} \times \mathcal{Y}}$.

**Definition**

The **empirical risk** of $f$ with respect to $\mathcal{D}_n$ is

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- The **unconstrained** empirical risk minimizer can overfit.
  - i.e. if we minimize $\hat{R}_n(f)$ over **all functions**, we overfit.

# Constrained Empirical Risk Minimization

**Definition**

A **hypothesis space** $\mathcal{F}$ is a set of functions mapping $\mathcal{X} \to \mathcal{Y}$.

- This is the collection of prediction functions we are choosing from.

- An **empirical risk minimizer** (ERM) in $\mathcal{F}$ is

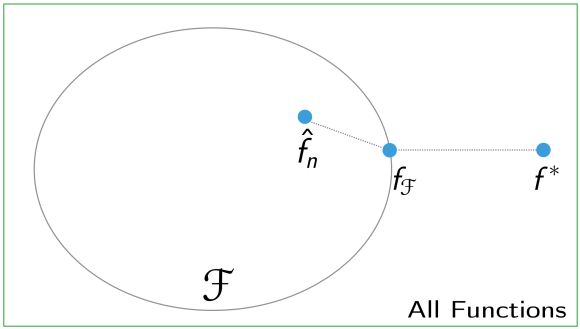
$$\hat{f}_n \in \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- From now on "ERM" always means "constrained ERM".
- So we should always specify the hypothesis space when we're doing ERM.

# Error Decomposition Review

- Excess risk decomposition for function $\tilde{f}_n$ returned by an optimization algorithm in practice:

$$\begin{aligned}\textbf{Excess Risk}(\tilde{f}_n) &= R(\tilde{f}_n) - R(f^*) \\ &= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}\end{aligned}$$



# ERM Overview

- Given a loss function $\ell$,
- Choose a hypothesis space $\mathcal{F}$.
- Use an optimization method to find an empirical risk minimizer $\hat{f}_n \in \mathcal{F}$:

$$\hat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- Or find a $\tilde{f}_n$ that comes close to $\hat{f}_n$
- The machine learning scientist's job:
  - Choose $\mathcal{F}$ that balances approximation and estimation error.
  - As we get more training data, we can use a bigger $\mathcal{F}$.

# Example: Linear Least Squares Regression

## Setup

- Loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- **Hypothesis space:** $\mathcal{F} = \left\{ f : \mathsf{R}^d \to \mathsf{R} \mid f(x) = w^T x,\, w \in \mathsf{R}^d \right\}$

- Given a data set $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$,
  - Our goal is to find the ERM $\hat{f} \in \mathcal{F}$.

# Example: Linear Least Squares Regression

## Objective Function: Empirical Risk

We want to find the function in $\mathcal{F}$, parametrized by $w \in \mathrm{R}^d$, that minimizes the empirical risk:

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \left( w^T x_i - y_i \right)^2$$

- How do we solve this optimization problem?

$$\min_{w \in \mathrm{R}^d} \hat{R}_n(w)$$

- (For OLS there's a closed form solution, but in general there isn't.)

# Gradient Descent

# Unconstrained Optimization

## Setting

We assume that the objective function $f : \mathrm{R}^d \to \mathrm{R}$ is *differentiable*.
We want to find

$$x^* = \arg\min_{x \in \mathrm{R}^d} f(x)$$

# The Gradient

- Let $f : \mathrm{R}^d \to \mathrm{R}$ be differentiable at $x_0 \in \mathrm{R}^d$.
- The **gradient** of $f$ at the point $x_0$, denoted $\nabla_x f(x_0)$, is the direction in which $f(x)$ **increases fastest**, if we start from $x_0$.
- The **gradient** of $f$ is the partial derivatives of all dimensions: $\nabla f(x) = [\partial f/\partial x_1(x), ..., \partial f/\partial x_d(x)]$.

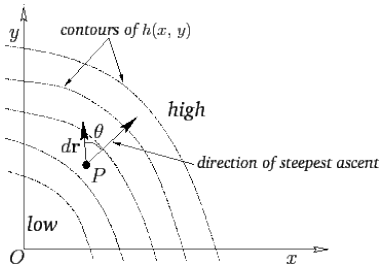



Figure A.111 from Newtonian Dynamics, by Richard Fitzpatrick.

# Gradient Descent

- To reach a local minimum as fast as possible, we want to go in the opposite direction from the gradient.

## Gradient Descent

- Initialize $x \leftarrow 0$.
- Repeat:
  - $x \leftarrow x - \eta \nabla f(x)$
- until the stopping criterion is satisfied.

- The "step size" $\eta$ is not the amount by which we update $x$!
- "Step size" is also referred to as "learning rate" in neural networks literature.

# Gradient Descent Path

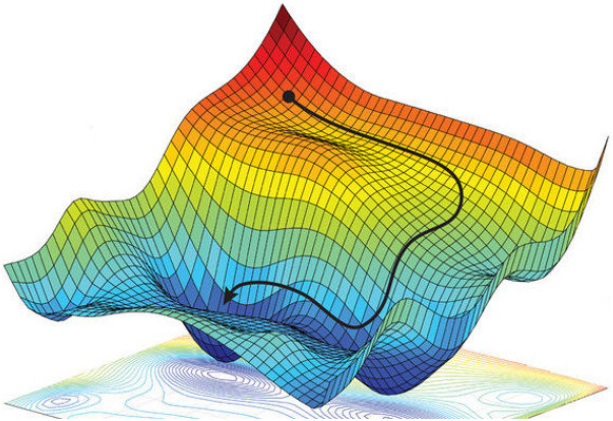
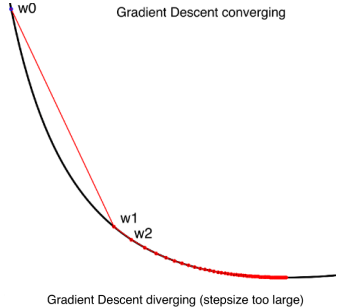


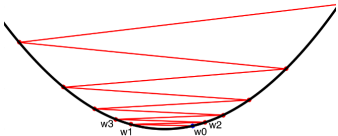
Image credit: Amini et al. Spatial Uncertainty Sampling for End-to-End Control. 2018.

# Gradient Descent: Step Size

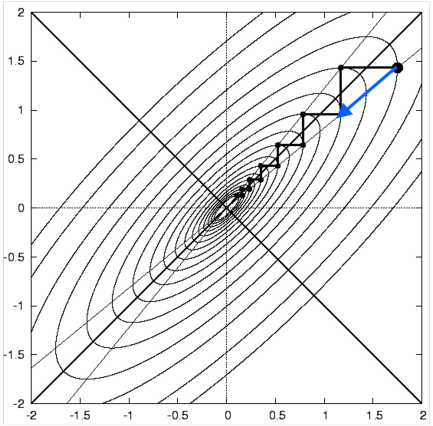
A fixed step size will work, eventually, as long as it's small enough

- If $\eta$ is too large, the optimization process might diverge
- In practice, it often makes sense to try several fixed step sizes
- Intuition on when to take big steps and when to take small steps?

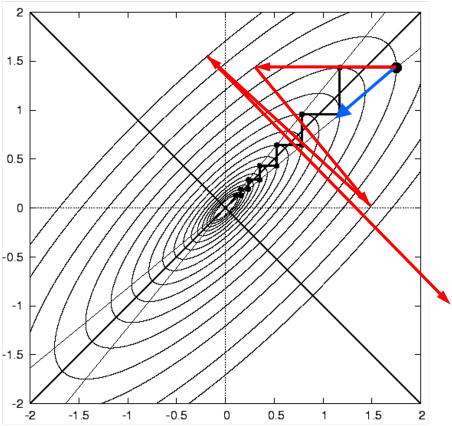


# 2D Divergence example




Small Step Size




Large Step Size

# Notes on Convergence

- Gradient descent with an appropriate step size converges to stationary point (derivative = 0) for differentiable functions.
- Stationary points can be (local) minima, (local) maxima, saddle points, etc.
- Gradient descent can converge to global minimum for **convex functions**.

# Convergence Theorem for Fixed Step Size

**Theorem**

*Suppose $f : \mathrm{R}^d \to \mathrm{R}$ is convex and differentiable, and $\nabla f$ is* ***Lipschitz continuous*** *with constant $L > 0$ (L-**smooth**), i.e.*

$$\|\nabla f(x) - \nabla f(x')\| \leqslant L\|x - x'\|$$

*for any $x, x' \in \mathrm{R}^d$. Then gradient descent with fixed step size $\eta \leqslant 1/L$* ***converges****. In particular,*

$$f(x^{(k)}) - f(x^*) \leqslant \frac{\|x^{(0)} - x^*\|^2}{2\eta k}.$$

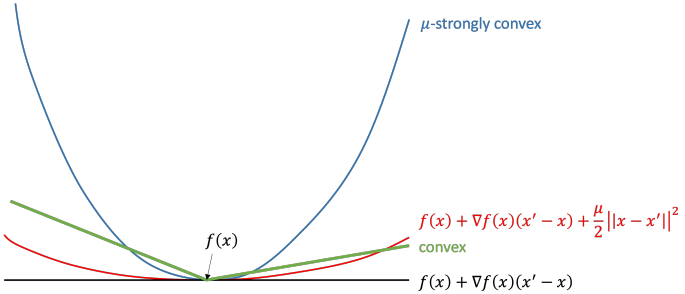
This says that gradient descent is guaranteed to converge and that it converges with rate $O(1/k)$.

# Strongly Convex Functions

## Definition

A function f is μ-strongly convex if

$$f(x') \geqslant f(x) + \nabla f(x) \cdot (x' - x) + \frac{\mu}{2}\|x - x'\|^2$$



# Convergence Theorem for Strongly Convex Functions

**Theorem**

*If $f$ is $L$-smooth and $\mu$-strongly convex, and step size $0 < \eta \leqslant \frac{1}{L}$, then gradient descent converges with the following inequality:*

$$\|x^{(k)} - x^*\|^2 \leqslant (1 - \eta\mu)^k \|x^{(0)} - x^*\|^2$$

This means we can get linear convergence, but it depends on $\mu$. If the estimate of $\mu$ is bad then the rate is not great.

# Gradient Descent: When to Stop?

- Wait until $\|\nabla f(x)\|_2 \leqslant \varepsilon$, for some $\varepsilon$ of your choosing.
  - (Recall $\nabla f(x) = 0$ at a local minimum.)
- **Early stopping:**
  - evalute loss on validation data (unseen held out data) after each iteration;
  - stop when the loss does not improve (or gets worse).

# Gradient Descent for Empirical Risk - Scaling Issues

# Quick recap: Gradient Descent for ERM

- We have a hypothesis space of functions $\mathcal{F} = \{f_w : \mathcal{X} \to \mathcal{Y} \mid w \in \mathbb{R}^d\}$
  - Parameterized by $w \in \mathbb{R}^d$.
- Finding an empirical risk minimizer entails finding a $w$ that minimizes

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_w(x_i), y_i)$$

- Suppose $\ell(f_w(x_i), y_i)$ is differentiable as a function of $w$.
- Then we can do gradient descent on $\hat{R}_n(w)$

# Gradient Descent: Scalability

- At every iteration, we compute the gradient at the current $w$:

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

- How does this scale with $n$?
- We have to iterate over all $n$ training points to take a single step. $[O(n)]$
- Can we make progress without looking at all the data before updating $w$?

# Stochastic Gradient Descent

# "Noisy" Gradient Descent

- Instead of using the gradient, we use a noisy estimate of the gradient.
- Turns out this can work just fine!
- **Intuition**:
  - Gradient descent is an iterative procedure anyway.
  - At every step, we have a chance to recover from previous missteps.

# Minibatch Gradient

- The **full gradient** is

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

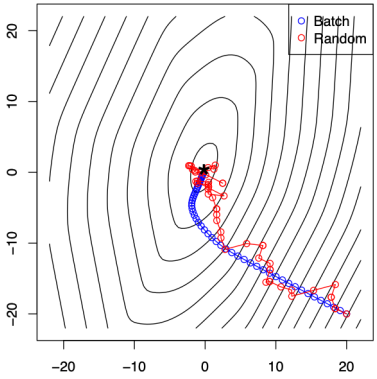
- It's an average over the **full batch** of data $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Let's take a random subsample of size $N$ (called a **minibatch**):

$$(x_{m_1}, y_{m_1}), \ldots, (x_{m_N}, y_{m_N})$$

- The **minibatch gradient is**

$$\nabla \hat{R}_N(w) = \frac{1}{N} \sum_{i=1}^{N} \nabla_w \ell(f_w(x_{m_i}), y_{m_i})$$

# Batch vs Stochastic Methods




(Slide adapted from Ryan Tibshirani)

Rule of thumb for stochastic methods:

- Stochastic methods work well far from the optimum
- But struggle close the the optimum

# Minibatch Gradient Properties

- The minibatch gradient is an **unbiased estimator** for the [full] batch gradient. What does that mean?

$$\mathbb{E}\left[\nabla \hat{R}_N(w)\right] = \nabla \hat{R}_n(w)$$

- The bigger the minibatch, the better the estimate.

$$\text{Var}\left[\nabla \hat{R}_N(w)\right] = \text{Var}\left[\frac{1}{N}\sum_i \nabla \hat{R}_i(w)\right] = \frac{1}{N^2}\text{Var}\left[\sum_i \nabla \hat{R}_i(w)\right] = \frac{1}{N}\text{Var}\left[\nabla \hat{R}_i(w)\right]$$

- Tradeoffs of minibatch size:
  - Bigger $N \implies$ Better estimate of gradient, but slower (more data to process)
  - Smaller $N \implies$ Worse estimate of gradient, but can be quite fast
- Because of vectorization, the computation cost of minibatches is sublinear

# Convergence of SGD

- For convergence guarantee, use **diminishing step sizes**, e.g. $\eta_k = 1/k$
- Theoretically, GD is much faster than SGD in terms of convergence rate and number of steps:
  - much faster to add a digit of accuracy (more details later)
  - costlier to compute a single step
  - but most of that advantage comes into play once we're already pretty close to the minimum
  - in many ML problems we don't care about optimizing to high accuracy (why?)

# Step Sizes in Minibatch Gradient Descent

## Minibatch Gradient Descent (minibatch size $N$)

- initialize $w = 0$
- repeat
  - randomly choose $N$ points $\{(x_i, y_i)\}_{i=1}^{N} \subset \mathcal{D}_n$
  - $w \leftarrow w - \eta \left[ \frac{1}{N} \sum_{i=1}^{N} \nabla_w \ell(f_w(x_i), y_i) \right]$

- For SGD, fixed step size can work well in practice.
- Typical approach: Fixed step size reduced by constant factor whenever validation performance stops improving (staircase decay).
- Other schedules: inverse time decay (1/t) etc.

# Convergence of SGD Theorem (Optional)

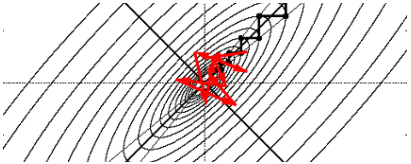
More on why we need a diminishing step size.

**Theorem**

*If $f$ is L-smooth and convex, and SGD has bounded variance $Var(\nabla f(x^{(k)})) \leqslant \sigma^2$ for all $k$, then SGD with step size $\eta \leqslant \frac{1}{L}$ satisifies:*

$$\min_k \mathbb{E}[\|\nabla f(x^{(k)})\|^2] \leqslant \frac{f(x^{(0)}) - f(x^*)}{\sum_k \eta_k} + \frac{L\sigma^2}{2} \frac{\sum_k \eta_k^2}{\sum_k \eta_k}$$

The extra term of variance will dominate if the step size does not decrease. [1]



[1] https://www.cs.ubc.ca/~schmidtm/Courses/540-W19/L11.pdf

# Summary

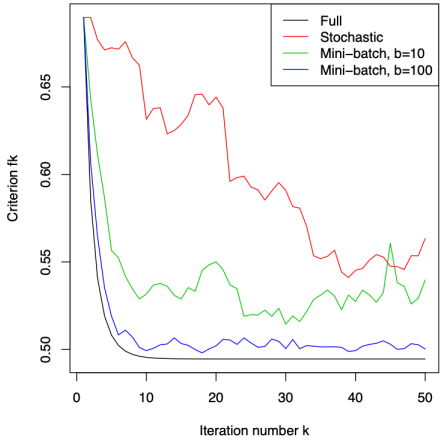
- **Gradient descent** or **"full-batch" gradient descent**
  - Use full data set of size $n$ to determine step direction
- **Minibatch gradient descent**
  - Use a **random** subset of size $N$ to determine step direction
- **Stochastic gradient descent**
  - Minibatch with $N = 1$.
  - Use a single randomly chosen point to determine step direction.

These days terminology isn't used so consistently, so when referring to SGD, always clarify the [mini]batch size.

SGD is much more efficient in time and memory cost and has been quite successful in large-scale ML.

# Example: Logistic regression with $\ell_2$ regularization

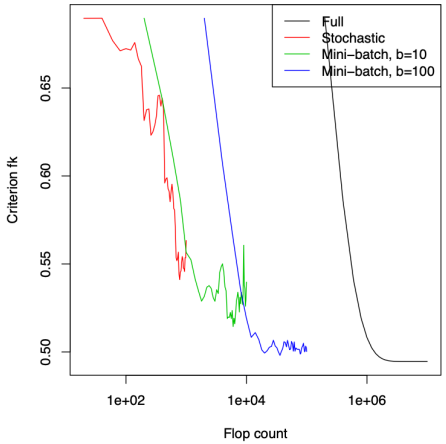
Batch methods converge faster :




(Example from Ryan Tibshirani)

# Example: Logistic regression with $\ell_2$ regularization

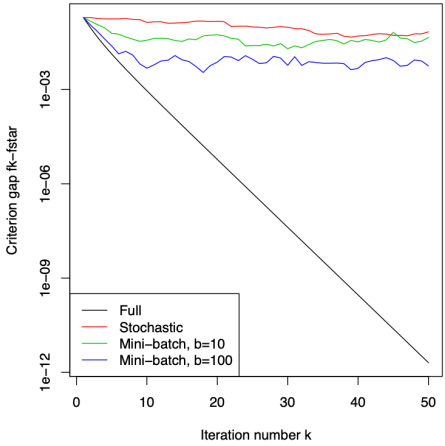
Stochastic methods are computationally more efficient:




(Example from Ryan Tibshirani)

# Example: Logistic regression with $\ell_2$ regularization

Batch methods are much faster close to the optimum:




(Example from Ryan Tibshirani)

# Loss Functions: Regression

# Regression Problems

- Examples:
  - Predicting the stock price given history prices
  - Predicting medical cost of given age, sex, region, BMI etc.
  - Predicting the age of a person based on their photos
- Notation:
  - $\hat{y}$ is the predicted value (the action)
  - $y$ is the actual observed value (the outcome)

# Loss Functions for Regression

- A loss function in general:
$$(\hat{y}, y) \mapsto \ell(\hat{y}, y) \in \mathrm{R}$$
- Regression losses usually only depend on the **residual** $r = y - \hat{y}$.
  - what you have to add to your prediction to get the correct answer.
- A loss $\ell(\hat{y}, y)$ is called **distance-based** if:
  1. It only depends on the residual:
  $$\ell(\hat{y}, y) = \psi(y - \hat{y}) \quad \text{for some } \psi{:}\mathrm{R} \to \mathrm{R}$$
  2. It is zero when the residual is 0:
  $$\psi(0) = 0$$

# Distance-Based Losses are Translation Invariant

- Distance-based losses are translation-invariant. That is,

$$\ell(\hat{y}+b, y+b) = \ell(\hat{y}, y) \qquad \forall b \in \mathrm{R}.$$

- When might you not want to use a translation-invariant loss?
- Sometimes the relative error $\frac{\hat{y}-y}{y}$ is a more natural loss (but not translation-invariant)

# Some Losses for Regression

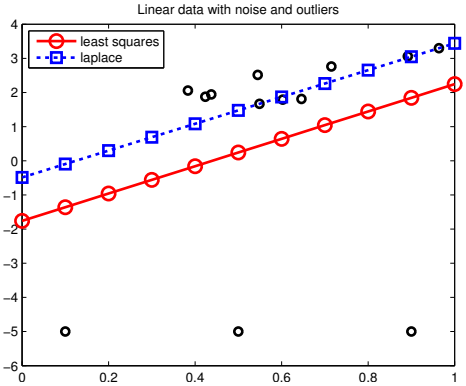
- **Residual:** $r = y - \hat{y}$
- **Square** or $\ell_2$ Loss: $\ell(r) = r^2$
- **Absolute** or **Laplace** or $\ell_1$ Loss: $\ell(r) = |r|$

| $y$ | $\hat{y}$ | $\lvert r\rvert = \lvert y - \hat{y}\rvert$ | $r^2 = (y - \hat{y})^2$ |
|---|---|---|---|
| 1 | 0 | 1 | 1 |
| 5 | 0 | 5 | 25 |
| 10 | 0 | 10 | 100 |
| 50 | 0 | 50 | 2500 |

- An outlier is a data point that differs significantly from other observations.
- Outliers typically have large residuals.
- Square loss much more affected by outliers than absolute loss.

# Loss Function Robustness

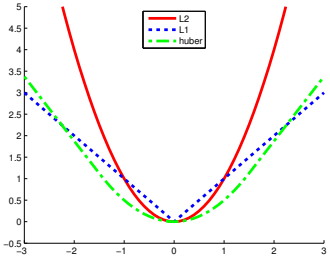
- **Robustness** refers to how affected a learning algorithm is by outliers.




KPM Figure 7.6

# Some Losses for Regression

- **Square** or $\ell_2$ Loss: $\ell(r) = r^2$ (*not robust*)
- **Absolute** or **Laplace** Loss: $\ell(r) = |r|$ (*not differentiable*)
  - gives **median regression**
- **Huber** Loss: Quadratic for $|r| \leqslant \delta$ and linear for $|r| > \delta$ (*robust and differentiable*)
  - Equal values and slopes at $r = \delta$




KPM Figure 7.6

# Classification Loss Functions

# The Classification Problem

- Examples:
  - Predict whether the image contains a cat
  - Predict whether the email is spam
- Classification spaces:
  - Input space $\mathrm{R}^d$
  - Outcome space $\mathcal{Y} = \{-1, 1\}$
- Inference:

$$f(x) > 0 \implies \text{Predict } 1$$
$$f(x) < 0 \implies \text{Predict } -1$$

How can we optimize the model output?

# The Score Function

- Output space $\mathcal{Y} = \{-1, 1\}$
- **Real-valued prediction function** $f : \mathcal{X} \to \mathrm{R}$

**Definition**

The value $f(x)$ is called the **score** for the input $x$.

- In this context, $f$ may be called a **score function**.
- The magnitude of the score can be interpreted as our **confidence of our prediction**.

# The Margin

**Definition**

The **margin** (or **functional margin**) for a predicted score $\hat{y}$ and the true class $y \in \{-1, 1\}$ is $y\hat{y}$.

- The margin is often written as $yf(x)$, where $f(x)$ is our score function.
- The margin is a measure of how **correct** we are:
  - If $y$ and $\hat{y}$ are the same sign, prediction is **correct** and margin is **positive**.
  - If $y$ and $\hat{y}$ have different sign, prediction is **incorrect** and margin is **negative**.
- We want to **maximize the margin**.
- Most classification losses depend only on the margin (they are **margin-based losses**).

# Classification Losses: $0-1$ Loss

- If $\tilde{f}$ is the inference function ($1$ if $f(x) > 0$ and $-1$ otherwise), then
- The **0-1 loss** for $f : \mathcal{X} \to \{-1, 1\}$:

$$\ell(f(x), y) = \mathbb{1}[\tilde{f}(x) \neq y]$$

- Empirical risk for $0-1$ loss:

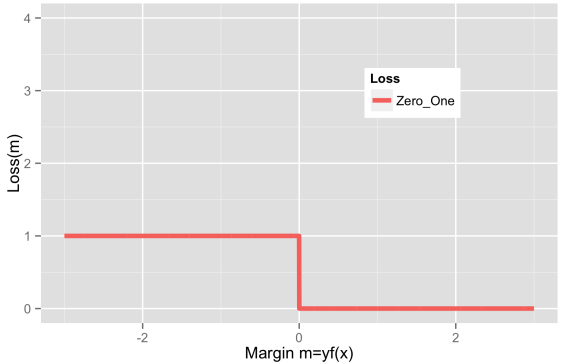
$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}[y_i f(x_i) \leqslant 0]$$

Minimizing empirical $0-1$ risk not computationally feasible.

$\hat{R}_n(f)$ is non-convex, not differentiable, and even discontinuous.

# Classification Losses

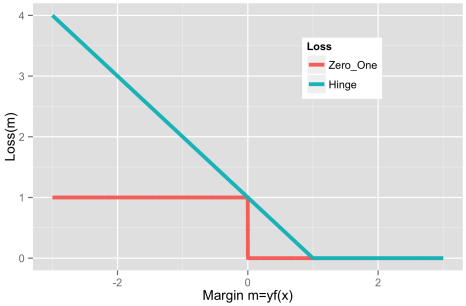
Zero-One loss: $\ell_{0\text{-}1} = \mathbb{1}[m \leqslant 0]$




- x-axis is **margin**: $m > 0 \iff$ correct classification

# Hinge Loss

SVM/Hinge loss: $\ell_{\text{Hinge}} = \max(1 - m, 0)$



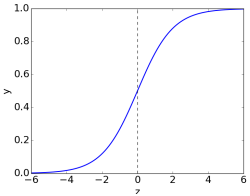

Hinge is a **convex**, **upper bound** on $0-1$ loss. Not differentiable at $m = 1$.

We will cover SVM and Hinge loss in more details in future lectures.

# Logistic Regression

- Also known as linear classification. Logistic regression is not actually "regression."
- Two equivalent types of logistic regression losses, depending on the labels.
- If the label is 0 or 1:
- $\hat{y} = \sigma(z)$, where $\sigma$ is the sigmoid function, and $z = f(x) = w^\top x$.

$$\sigma(z) = \frac{1}{1+\exp(-z)}$$



# Logistic Regression

- If the label is 0 or 1:
- $\hat{y} = \sigma(z)$, where $\sigma$ is the sigmoid function.

$$\sigma(z) = \frac{1}{1+\exp(-z)}$$

- The loss is binary cross entropy:

$$\ell_{\text{Logistic}} = -y \log(\hat{y}) - (1-y) \log(1-\hat{y})$$

- Remember the negative sign!

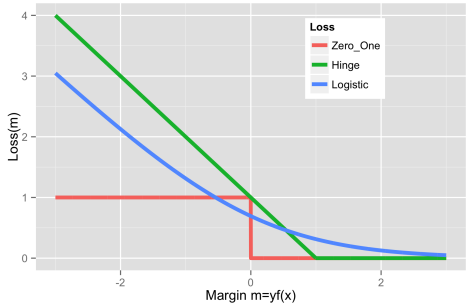
# Logistic Regression

- If the label is -1 o 1:
- Note: $1-\sigma(z)=\sigma(-z)$
- Now we can derive an equivalent loss form:

$$\begin{aligned}\ell_{\text{Logistic}} &= \begin{cases} -\log(\sigma(z)) & \text{if} \quad y=1 \\ -\log(\sigma(-z)) & \text{if} \quad y=-1 \end{cases} \\ &= -\log(\sigma(yz)) \\ &= -\log(\frac{1}{1+e^{-yz}}) \\ &= \log(1+e^{-m}).\end{aligned}$$

# Logistic Loss

Logistic/Log loss: $\ell_{\text{Logistic}} = \log\left(1 + e^{-m}\right)$



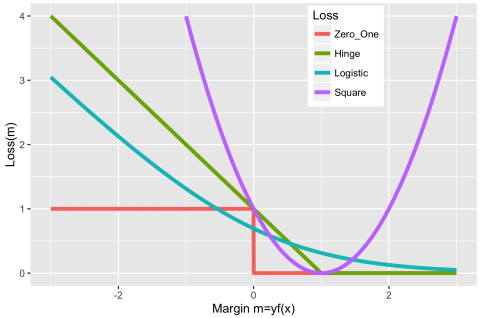

Logistic loss is differentiable. Logistic loss always rewards a larger margin (the loss is never 0).

# What About Square Loss for Classification?

- Loss $\ell(f(x), y) = (f(x) - y)^2$.
- Turns out, can write this in terms of margin $m = f(x)y$:
- Using fact that $y^2 = 1$, since $y \in \{-1, 1\}$.

$$\begin{aligned} \ell(f(x), y) &= (f(x) - y)^2 \\ &= f^2(x) - 2f(x)y + y^2 \\ &= f^2(x)y^2 - 2f(x)y + 1 \\ &= (1 - f(x)y)^2 \\ &= (1 - m)^2 \end{aligned}$$

# What About Square Loss for Classification?




Heavily penalizes outliers (e.g. mislabeled examples).

# Summary

- Gradient descent: step size/learning rate, batch size, convergence
- Loss functions for regression and classification problems.
- Regression: Squared (L2) loss, Absolute (L1) loss, Huber loss.
- Classification: Hinge loss, Logistic loss.
- Residual, margin
- Logistic regression