# Loss Functions for Regression and Classification

David S. Rosenberg

New York University

February 6, 2018

# Contents

# Regression Loss Functions

# Regression Notation

- Regression spaces:
  - Input space $\mathcal{X} = \mathbf{R}^d$
  - Action space $\mathcal{A} = \mathbf{R}$
  - Outcome space $\mathcal{Y} = \mathbf{R}$.
- Since $\mathcal{A} = \mathcal{Y}$, we can use more traditional notation:
  - $\hat{y}$ is the predicted value (the action)
  - $y$ is the actual observed value (the outcome)

# Loss Functions for Regression

- In general, loss function may take the form

$$(\hat{y}, y) \mapsto \ell(\hat{y}, y) \in \mathbf{R}$$

- Regression losses usually only depend on the **residual** $r = y - \hat{y}$.
    - what you have to add to your prediction to get the right answer
- Loss $\ell(\hat{y}, y)$ is called **distance-based** if it
    1. only depends on the residual:

    $$\ell(\hat{y}, y) = \psi(y - \hat{y}) \quad \text{for some } \psi : \mathbf{R} \to \mathbf{R}$$

    2. loss is zero when residual is 0:

    $$\psi(0) = 0$$

# Distance-Based Losses are Translation Invariant

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

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

- When might you not want to use a translation-invariant loss?
- Sometimes relative error $\frac{\hat{y}-y}{y}$ is a more natural loss (but not translation-invariant)
- Often you can transform response $y$ so it's translation-invariant (e.g. log transform)

# Some Losses for Regression

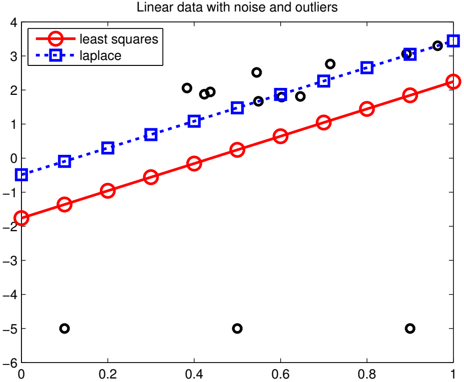
- **Residual:** $r = y - \hat{y}$
- **Square** or $\ell_2$ Loss: $\ell(r) = r^2$
- **Absolute** or **Laplace** or $\ell_1$ Loss: $\ell(r) = |r|$

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

- Outliers typically have large residuals.
- Square loss much more affected by outliers than absolute loss.

# Loss Function Robustness

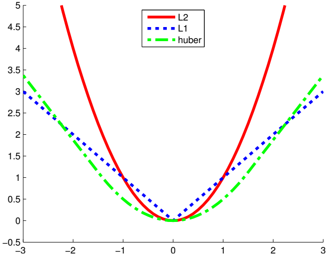
- **Robustness** refers to how affected a learning algorithm is by outliers.




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*)




- x-axis is the residual $y - \hat{y}$.

KPM Figure 7.6

# Classification Loss Functions

# The Classification Problem

- Outcome space $\mathcal{Y} = \{-1, 1\}$
- Action space $\mathcal{A} = \{-1, 1\}$
- **0-1 loss** for $f : \mathcal{X} \to \{-1, 1\}$:
$$\ell(f(x), y) = 1(f(x) \neq y)$$
- But let's allow **real-valued predictions** $f : \mathcal{X} \to \mathbf{R}$:
$$\begin{aligned} f(x) > 0 &\implies \text{Predict } 1 \\ f(x) < 0 &\implies \text{Predict } -1 \end{aligned}$$

# The Score Function

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

### Definition

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

- In this context, $f$ may be called a **score function**.
- Intuitively, magnitude of the score represents the **confidence of our prediction**.

### Definition

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

- The margin often looks like $yf(x)$, 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**.

# Margin-Based Losses

- Most classification losses depend only on the margin.
- Such a loss is called a **margin-based loss**.
- (There is a related concept, the **geometric margin**, in the notes on hard-margin SVM.)

# Classification Losses: $0-1$ Loss

- Empirical risk for $0-1$ loss:

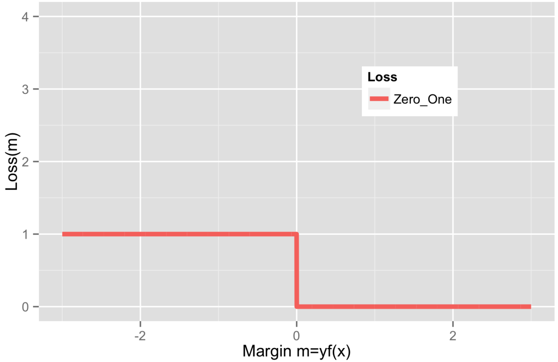
$$\hat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} 1(y_i f(x_i) \leqslant 0)$$

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

$\hat{R}_n(f)$ is non-convex, not differentiable (in fact, discontinuous!).
Optimization is **NP-Hard**.

# Classification Losses

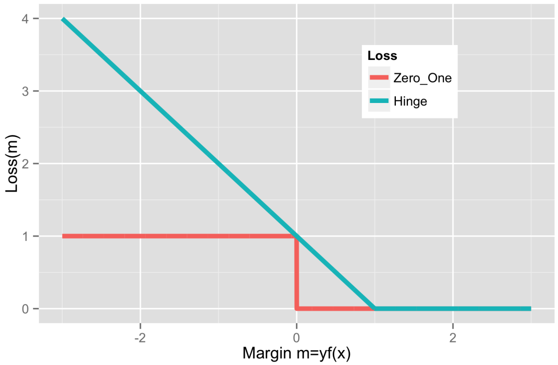
Zero-One loss: $\ell_{0\text{-}1} = 1(m \leqslant 0)$




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

# Classification Losses

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 have a "**margin error**" when $m<1$.

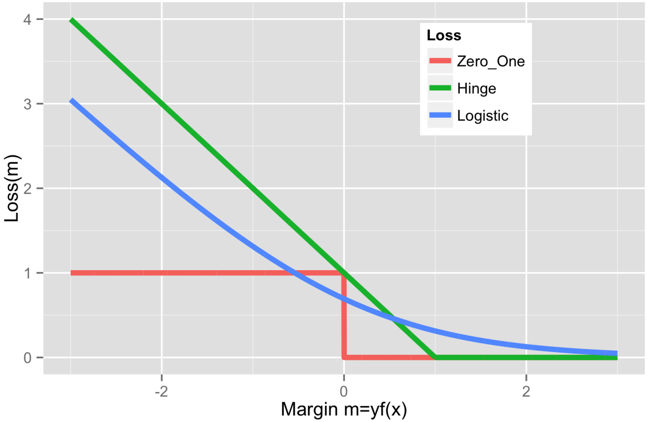
# (Soft Margin) Linear Support Vector Machine

- Hypothesis space: $\mathcal{F} = \left\{ f_w(x) = w^T x \mid w \in \mathbf{R}^d \right\}$.
- Loss: $\ell(m) = \max(1-m, 0)$ [**Hinge loss** – sometimes called **SVM loss**]
- Regularization: $\ell_2$

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \max\left(1 - y_i f_w(x_i), 0\right) + \lambda \|w\|_2^2$$

# Classification Losses

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




Logistic loss is differentiable. Logistic loss always wants more margin (loss never 0).

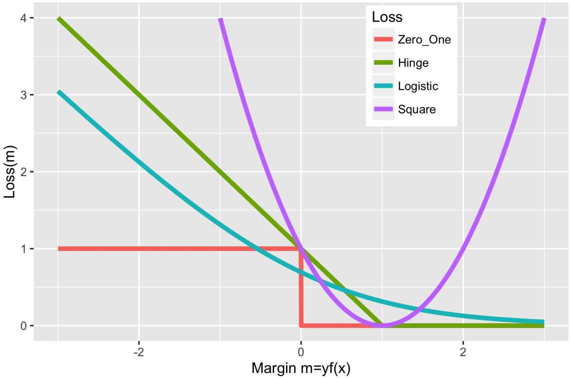
# What About Square Loss for Classification?

- Action space $\mathcal{A} = \mathbf{R}$ Output space $\mathcal{Y} = \{-1, 1\}$
- Loss $\ell(f(x), y) = (f(x) - y)^2$.
- Turns out, can write this in terms of margin $m = f(x)y$:

$$\ell(f(x), y) = (f(x) - y)^2 = (1 - f(x)y)^2 = (1 - m)^2$$

- Prove using fact that $y^2 = 1$, since $y \in \{-1, 1\}$.

# What About Square Loss for Classification?




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

<u>May have higher sample compl</u>exity (i.e. needs more data) than hinge & logistic[1].

[1] Rosasco et al's "Are Loss Functions All the Same?" http://web.mit.edu/lrosasco/www/publications/loss.pdf