Empirical Risk Minimization (ERM)

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- Definition
 - Recap
 - Background
 - Empirical Risk Minimization
- Binary Classification Loss Functions
- Regression Loss Functions
- Regularizers
- Famous Special Cases

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Recap

Remember the unconstrained SVM Formulation

$$\min_{\mathbf{w}} C \underbrace{\sum_{i=1}^{n} \max[1 - y_{i}(\mathbf{w}^{\top}\mathbf{x}_{i} + b), 0]}_{Hinge-Loss} + \underbrace{\|\mathbf{w}\|_{z}^{2}}_{l_{2}-Regularizer}$$

The hinge loss is the SVM's error function of choice, whereas the ℓ 2-regularizer reflects the complexity of the solution, and penalizes complex solutions. This is an example of empirical risk minimization with a loss function ℓ and a regularizer r,

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} \underbrace{I(h_{\mathbf{w}}(\mathbf{x}_{i}), y_{i})}_{Loss} + \underbrace{\lambda r(\mathbf{w})}_{Regularizer},$$

where the loss function is a continuous function which penalizes training error, and the regularizer is a continuous function which penalizes classifier complexity. Here, we define λ as $\frac{1}{C}$ from the previous lecture.

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4 / 28

Background

- Consider the following situation, a general setting of many supervised learning problems.
- We have two spaces of objects X and Y and would like to learn a function $h: X \to Y$ which outputs an object $y \in Y$, given $x \in X$.
- To do so, we have at our disposal a training set of n examples $(x_1, y_1), ..., (x_n, y_n)$ where $x_i \in X$ is an input and $y_i \in Y$ is the corresponding response that we wish to get from $h(x_i)$.
- To put it more formally, we assume that there is a **joint probability distribution** p(x,y) over X and Y, and that the training set consists of n instances $(x_1,y_1),...,(x_n,y_n)$ drawn i.i.d. from p(x,y).
- Note that the assumption of a joint probability distribution allows us to model uncertainty in predictions because y is not a deterministic function of x, but rather a random variable with conditional distribution p(x|y) for a fixed x.

Background

We also assume that we are given a **non-negative real-valued loss function** $L(\widehat{y}, y)$ which measures how different the prediction \widehat{y} of a hypothesis is from the true outcome y. The risk associated with hypothesis h(x) is then defined as the expectation of the loss function:

$$R(h) = E[L(h(x), y)] = \int L(h(x), y) dP(x, y)$$

A loss function commonly used in theory is the 0-1 loss function: $L(\widehat{y}, y) = I(\widehat{y} \neq y)$, where $I(\cdot)$ is the indicator notation.

The ultimate goal of a learning algorithm is to find a hypothesis h^* among a fixed class of functions H for which the risk R(h) is minimal:

$$h^* = \underset{h \in H}{\operatorname{arg\,min}} R(h).$$

6 / 28

Empirical Risk Minimization

In general, the risk R(h) cannot be computed because the distribution P(x,y) is unknown to the learning algorithm (this situation is referred to as agnostic learning). However, we can compute an approximation, called empirical risk, by averaging the loss function on the training set:

$$R_{emp}(h) = \frac{1}{n} \sum_{i=1}^{n} L(h(x_i), y_i).$$

The empirical risk minimization principle states that the learning algorithm should choose a hypothesis \hat{h} which minimizes the empirical risk:

$$h^* = \underset{h \in H}{\operatorname{arg\,min}} R(h).$$

Thus **Empirical Risk Minimization (ERM)** is a principle in statistical learning theory which defines a family of learning algorithms and is used to give theoretical bounds on their performance.

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7 / 28

- Definition
 - Recap
 - Background
 - Empirical Risk Minimization
- Binary Classification Loss Functions
- Regression Loss Functions
- 4 Regularizers
- Famous Special Cases

Binary Classification Loss Functions

Different Machine Learning algorithms use different loss functions

Table 1: Binary Classification Loss Functions, $y \in \{-1, +1\}$

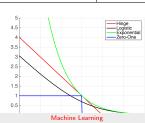
Loss $\ell(h_{\mathbf{w}}(\mathbf{x}_i, y_i))$	Usage	Comments
Hinge-Loss: $\max [1 - h_{\mathbf{w}}(\mathbf{x}_i)y_i, 0]^p$	• Standard SVM($p = 1$) • (Differentiable) Squared Hingeless SVM ($p = 2$)	When used for Standard SVM, the loss function denotes the size of the margin between linear separator and its closest points in either class. Only differentiable everywhere with $p=2$.
Log-Loss: $\log(1 + e^{-h_{\mathbf{W}}(\mathbf{x}_i)y_i})$	Logistic Regression	One of the most popular loss functions in Machine Learning, since its outputs are well-calibrated probabilities.



Binary Classification Loss Functions

Table 1: Binary Classification Loss Functions, $y \in \{-1, +1\}$

Loss $\ell(h_{w}(x_i,y_i))$	Usage	Comments
Exponential Loss: $e^{-h_{\mathbf{w}}(\mathbf{x}_i)y_i}$	AdaBoost	This function is very aggressive. The loss of a mis-prediction increases <i>exponentially</i> with the value of $-h_{\mathbf{w}}(\mathbf{x}_i)y_i$. This can lead to nice convergence results, for example in the case of Adaboost, but it can also cause problems with noisy data.
Zero-One Loss: $\delta(\operatorname{sign}(h_{\mathbf{w}}(\mathbf{x}_i)) \neq y_i)$	Actual Classification Loss	Non-continuous and thus impractical to optimize.



Binary Classification Loss Functions

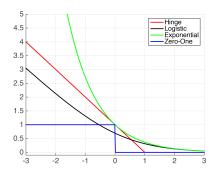


Figure 1: Plots of Common Classification Loss Functions. x-axis: $h(\mathbf{x}_i)y_i$, or "correctness" of prediction; y-axis: loss value

Quiz: Which functions are strict upper bounds on the 0/1-loss?

Quiz: What can you say about the hinge-loss and the log-loss as $z \to -\infty$?

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- Definition
 - Recap
 - Background
 - Empirical Risk Minimization
- Binary Classification Loss Functions
- Regression Loss Functions
- 4 Regularizers
- Famous Special Cases

Regression Loss Functions

Loss for regression algorithms (a prediction can lie anywhere on the real-number line):

Table 2: Regression Loss Functions, $\,y\in\mathbb{R}\,$

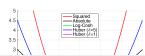
Loss $\ell(h_{\mathbf{w}}(\mathbf{x}_i, y_i))$	Comments
	Most popular regression loss function
	• Estimates <u>Mean</u> Label
Squared Loss: $(h(x_i) - y_i)^2$	Also known as Ordinary Least Squares (OLS)
	DISADVANTAGE: Somewhat sensitive to outliers/noise
	Also a very popular loss function
	• Estimates <u>Median</u> Label
Absolute Loss: $ h(x_i) - y_i $	ADVANTAGE: Less sensitive to noise
	DISADVANTAGE: Not differentiable at 0

13 / 28

Regression Loss Functions

Table	2:Regression	Loss	Functions,	У	\in	\mathbb{R}

Loss $\ell(h_{\mathbf{w}}(\mathbf{x}_i, y_i))$	Comments
Huber Loss: • $\frac{1}{2}(h(\mathbf{x}_i) - y_i)^2$ if $ h(\mathbf{x}_i) - y_i < \delta$, • otherwise $\delta(h(\mathbf{x}_i) - y_i - \frac{\delta}{2})$	 Also known as Smooth Absolute Loss Once-differentiable Takes on behavior of Squared-Loss when loss is small, and Absolute Loss when loss is large. ADVANTAGE: "Best of Both Worlds" of Squared and Absolute Loss
Log-Cosh Loss: $log(cosh(h(\mathbf{x}_i) - y_i)),$ $cosh(x) = \frac{e^x + e^{-x}}{2}$	ADVANTAGE: Similar to Huber Loss, but twice dif- ferentiable everywhere



14 / 28

Machine Learning

Regression Loss Functions

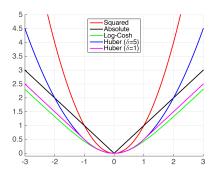


Figure 2: Plots of Common Regression Loss Functions - x-axis: $h(x_i)y_i$, or "error" of prediction; y-axis: loss value

Quiz: What do the loss functions in Table 2 look like with respect to $z = h(\mathbf{x}_i) - y_i$?

- Definition
 - Recap
 - Background
 - Empirical Risk Minimization
- Binary Classification Loss Functions
- Regression Loss Functions
- 4 Regularizers
- Famous Special Cases

- In mathematics, statistics, and computer science, particularly in machine learning problems, regularization is the process of adding information in order to solve an ill-posed problem or to prevent overfitting.
- When we look at regularizers it helps to change the formulation of the optimization problem to obtain a better geometric intuition.
- In previous sections, I₂-regularizer has been introduced as the component in SVM that reflects the complexity of solutions.

Besides the $\it l_2$ -regularizer, other types of useful regularizers and their properties are listed in the following Table.

Table 3:Types of Regularizers

Regularizer $r(\mathbf{w})$	Properties
l_2 -Regularization $r(\mathbf{w}) = \mathbf{w}^{\top} \mathbf{w} = \ \mathbf{w}\ _2^2$	 ADVANTAGE: Strictly Convex; Differentiable DISADVANTAGE: Uses weights on all features, i.e. relies on all features to some degree (ideally we would like to avoid this) - these are known as <u>Dense Solutions</u>.
$egin{aligned} & I_1 ext{-Regularization} \ & r(\mathbf{w}) = \ \mathbf{w}\ _1 \end{aligned}$	 Convex (but not strictly) DISADVANTAGE: Not differentiable at 0 (the point which minimization is intended to bring us to Effect: Sparse (i.e. not Dense) Solutions

Table 3:Types of Regularizers

Regularizer $r(\mathbf{w})$	Properties
$I_p ext{-Norm} \ \mathbf{w}\ _p = (\sum\limits_{i=1}^d v_i^p)^{1/p}$	 (often 0 Initialization dependent ADVANTAGE: Very sparse solutions DISADVANTAGE: Non-convex; Not differentiable
Elastic Net: $\alpha \ \mathbf{w}\ _1 + (1-\alpha) \ \mathbf{w}\ _2^2$ $\alpha \in [0,1)$	 ADVANTAGE: Strictly convex (i.e. unique solution) ADVANTAGE: Sparsity inducing (good for feature selection);Dual of squared-loss SVM, see SVEN DISADVANTAGE: Non-differentiable





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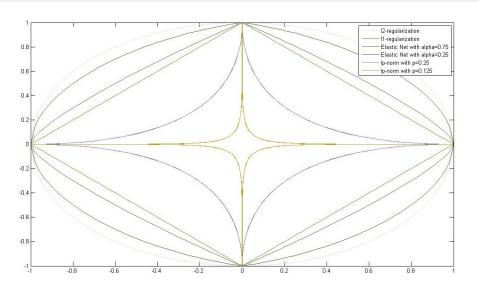


Figure 3: Plots of Common Regularizers

- Definition
 - Recap
 - Background
 - Empirical Risk Minimization
- 2 Binary Classification Loss Functions
- Regression Loss Functions
- 4 Regularizers
- Famous Special Cases

This section includes several special cases that deal with risk minimization, such as Ordinary Least Squares, Ridge Regression, Lasso, and Logistic Regression. The following blocks provide information on their loss functions, regularizers, as well as solutions.

Ordinary Least Squares

In statistics, ordinary least squares (OLS) is a type of linear least squares method for estimating the unknown parameters in a linear regression model.

goal:

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^{\top} x_i - y_i)^2$$

- Squared Loss
- No Regularization
- Closed form solution: $\mathbf{w} = (\mathbf{X}\mathbf{X}^{\top})^{-1}\mathbf{X}\mathbf{y}^{\top}, \mathbf{X} = [\mathbf{x}_1, ..., \mathbf{x}_n], \mathbf{y} = [y_1, ..., y_n]$
- There is an interesting connection between OLS and the first principal component of PCA (Principal Component Analysis). PCA also minimizes square loss, but looks at perpendicular loss (the horizontal distance between each point and the regression

Ridge Regression

Tikhonov regularization, is the most commonly used method of regularization of ill-posed problems. In statistics, the method is known as **ridge regression**.

goal:

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^{\top} x_i - y_i)^2 + \lambda \|\mathbf{w}\|_2^2$$

- Squared Loss
- I₂-Regularization
- $\mathbf{w} = (\mathbf{X}\mathbf{X}^{\top} + \lambda \mathbb{I})^{-1}\mathbf{X}\mathbf{y}^{\top}$
- Fast if data isn't too high dimensional
- Just 1 line of Julia / Python

Lasso

LASSO is a regression analysis method that performs both variable selection and regularization in order to enhance the prediction accuracy and interpretability of the statistical model it produces.

Goal:

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^{\top} \mathbf{x}_i - y_i)^2 + \lambda \|\mathbf{w}\|_1$$

- ADVANTAGE sparsity inducing (good for feature selection); Convex
- DISADVANTAGE Not strictly convex (no unique solution); Not differentiable (at 0)
- Solve with (sub)-gradient descent or SVEN

Elastic Net

Goal

$$\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^{\top} \mathbf{x}_{i} - y_{i})^{2} + \alpha \|\mathbf{w}\|_{1} + (1 - \alpha) \|\mathbf{w}\|_{2}^{2}$$

$$\alpha \in [0, 1)$$

- ADVANTAGE: Strictly convex (i.e. unique solution)
- +Sparsity inducing (good for feature selection)
- +Dual of squared-loss SVM, see SVEN
- DISADVANTAGE Non-differentiable
- Solve with (sub)-gradient descent or SVEN

Logistic Regression

In regression analysis, **logistic regression** is estimating the parameters of a logistic model; it is a form of binomial regression.

goal:

$$\min_{\mathbf{w},b} \frac{1}{n} \sum_{i=1}^{n} \log \left(1 + e^{-y_i(\mathbf{w}^{\top} \mathbf{x}_i + b)}\right)$$

- ullet Often I_1 or I_2 regularized
- Solve with gradient descent.
- $Pr(y|x) = \frac{1}{1+e^{-y(\mathbf{w}^\top x + b)}}$

Linear Support Vector Machine

goal:

$$\min_{\mathbf{w},b} C \sum_{i=1}^n \max[1-y_i(\mathbf{w}^{\top}\mathbf{x}_i+b),0] + \|\mathbf{w}\|_2^2$$

- Typically l_2 regularized (sometimes l_1).
- Quadratic program.
- When kernelized leads to sparse solutions.
- Kernelized version can be solved very efficiently with specialized algorithms (e.g. SMO)

The End