# Lecture 2 - Learning Binary & Multi-class Classifiers from Labelled Training Data

DD2424

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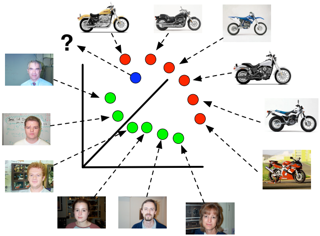
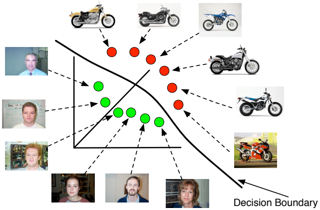
## Binary classification problem given labelled training data

Have labelled training examples




Given a test example how do we decide its class?

## High level solution




**Learn a decision boundary from the labelled training data.**

Compare the test example to the decision boundary.

## Technical description of the binary problem

- Have a set of labelled training examples

  $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ with each $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \{-1, 1\}$.

- Want to learn from $\mathcal{D}$ a classification function

$$g : \underset{\substack{\uparrow \\ \text{input space}}}{\mathbb{R}^d} \times \underset{\substack{\uparrow \\ \text{parameter space}}}{\mathbb{R}^p} \rightarrow \{-1, 1\}$$

  Usually

$$g(\mathbf{x}; \boldsymbol{\theta}) = \text{sign}(f(\mathbf{x}; \boldsymbol{\theta})) \quad \text{where} \quad f : \mathbb{R}^d \times \mathbb{R}^p \rightarrow \mathbb{R}$$

- Have to decide on
  1. Form of $f$ (a hyperplane?) and
  2. How to estimate $f$'s parameters $\hat{\boldsymbol{\theta}}$ from $\mathcal{D}$.

## Learn decision boundary discriminatively

- Set up an optimization of the form (usually)

$$\arg\min_{\boldsymbol{\theta}} \overbrace{\sum_{(\mathbf{x},y)\in\mathcal{D}} l(y, f(\mathbf{x};\boldsymbol{\theta}))}^{\text{training error}} + \lambda \underbrace{R(\boldsymbol{\theta})}_{\substack{\uparrow \\ \text{regularization term}}}$$

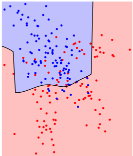
where

- $l(y, f(\mathbf{x} \mid \boldsymbol{\theta}))$ is the **loss function** and measures how well (and robustly) $f(\mathbf{x};\boldsymbol{\theta})$ predicts the label $y$.
- The **training error** term measures how well and robustly the function $f(\cdot\,;\boldsymbol{\theta})$ predicts the labels over all the training data.
- The **regularization** term measures the *complexity* of the function $f(\cdot\,;\boldsymbol{\theta})$.

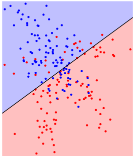
  Usually want to learn simpler functions $\Longrightarrow$ less risk of over-fitting.

# Comment on Over- and Under-fitting

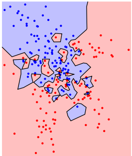
## Example of Over and Under fitting



**Bayes' Optimal**

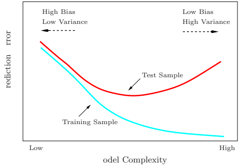


**Under-fitting**



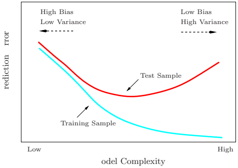
**Over-fitting**

## Overfitting




- Too much fitting $\Longrightarrow$ adapt too closely to the training data.
- Have a high variance predictor.
- This scenario is termed **overfitting**.
- In such cases predictor loses the ability to generalize.

## Underfitting




- Low complexity model $\implies$ predictor may have large bias
- Therefore predictor has poor generalization.

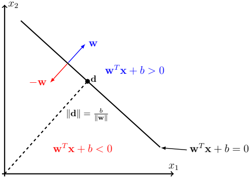
# Linear Decision Boundaries

## Linear discriminant functions

Linear function for the binary classification problem:

$$f(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$$

where model parameters are $\mathbf{w}$ the weight vector and $b$ the bias.




$$g(\mathbf{x}; \mathbf{w}, b) = \begin{cases} 1 & \text{if } f(\mathbf{x}; \mathbf{w}, b) > 0 \\ -1 & \text{if } f(\mathbf{x}; \mathbf{w}, b) < 0 \end{cases}$$

## Pros & Cons of Linear classifiers

**Pros**

- Low variance classifier
- Easy to estimate.

  Frequently can set up training so that have an easy optimization problem.
- For high dimensional input data a linear decision boundary can sometimes be sufficient.

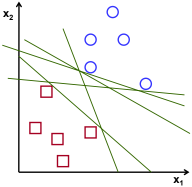
**Cons**

- High bias classifier

  Often the decision boundary is not well-described by a linear classifier.

## How do we choose & learn the linear classifier?






Given labelled training data:

*how do we choose and learn the best **hyperplane** to separate the two classes?*

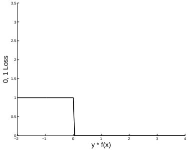
Have a linear classifier next need to decide:

1. How to measure the quality of the classifier w.r.t. labelled training data?
   - Choose/Define a **loss function**.

## Most intuitive loss function



**0, 1 Loss function**




For a single example $(\mathbf{x}, y)$ the 0-1 loss is defined as

$$l(y, f(\mathbf{x};\boldsymbol{\theta})) = \begin{cases} 0 & \text{if } y = \operatorname{sgn}(f(\mathbf{x};\boldsymbol{\theta})) \\ 1 & \text{if } y \neq \operatorname{sgn}(f(\mathbf{x};\boldsymbol{\theta})) \end{cases}$$

$$= \begin{cases} 0 & \text{if } y\, f(\mathbf{x};\boldsymbol{\theta}) > 0 \\ 1 & \text{if } y\, f(\mathbf{x};\boldsymbol{\theta}) < 0 \end{cases}$$

(assuming $y \in \{-1, 1\}$)

Applied to all training data $\Longrightarrow$ count the number of misclassifications.

Not really used in practice as has lots of problems! What are some?

Have a linear classifier next need to decide:

1. How to measure the quality of the classifier w.r.t. labelled training data?
   - Choose/Define a **loss function**.
2. How to measure the complexity of the classifier?
   - Choose/Define a **regularization** term.

## Most common regularization function

$L_2$ **regularization**

$$R(\mathbf{w}) = \|\mathbf{w}\|^2 = \sum_{i=1}^{d} w_i^2$$

Adding this form of regularization:

- Encourages $\mathbf{w}$ not to contain entries with large absolute values.
- or want small absolute values in all entries of $\mathbf{w}$.

## Supervised learning of my classifier

Have a linear classifier next need to decide:

1. How to measure the quality of the classifier w.r.t. labelled training data?
   - Choose/Define a **loss function**.
2. How to measure the complexity of the classifier?
   - Choose/Define a **regularization** term.
3. How to do estimate the classifier's parameters by optimizing relative to the above factors?

## Example: Squared Error loss

## Squared error loss & no regularization

- Learn $\mathbf{w}, b$ from $\mathcal{D}$. Find the $\mathbf{w}, b$ that minimizes:

$$L(\mathcal{D}, \mathbf{w}, b) = \frac{1}{2} \sum_{(\mathbf{x},y)\in\mathcal{D}} l_{\text{sq}}(y, f(\mathbf{x}; \mathbf{w}, b))$$
$$= \frac{1}{2} \sum_{(\mathbf{x},y)\in\mathcal{D}} \underbrace{\left((\mathbf{w}^T\mathbf{x} + b) - y\right)^2}_{\text{Squared error loss}}$$

  $L$ is known as the sum-of-squares error function.

- The $\mathbf{w}^*, b^*$ that minimizes $L(\mathcal{D}, \mathbf{w}, b)$ is known as the **Minimum Squared Error** solution.

- This minimum is found as follows....

## Technical interlude: Matrix Calculus



- Have a function $f : \mathbb{R}^d \to \mathbb{R}$ that is $f(\mathbf{x}) = b$
- We use the notation

$$\frac{\partial f}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_d} \end{pmatrix}$$

- **Example**: If $f(\mathbf{x}) = \mathbf{a}^T\mathbf{x} = \sum_{i=1}^{d} a_i x_i$ then

$$\frac{\partial f}{\partial x_i} = a_i \quad \Longrightarrow \quad \frac{\partial f}{\partial \mathbf{x}} = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix} = \mathbf{a}$$



- Have a function $f : \mathbb{R}^{d\times d} \to \mathbb{R}$ that is $f(X) = b$ with $X \in \mathbb{R}^{d\times d}$
- We use the notation

$$\frac{\partial f}{\partial X} = \begin{pmatrix} \frac{\partial f}{\partial x_{11}} & \frac{\partial f}{\partial x_{12}} & \cdots & \frac{\partial f}{\partial x_{1d}} \\ \frac{\partial f}{\partial x_{21}} & \frac{\partial f}{\partial x_{22}} & \cdots & \frac{\partial f}{\partial x_{2d}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial x_{d1}} & \frac{\partial f}{\partial x_{d2}} & \cdots & \frac{\partial f}{\partial x_{dd}} \end{pmatrix}$$

- **Example**: If $f(X) = \mathbf{a}^T X \mathbf{b} = \sum_{i=1}^{d} a_i \sum_{j=1}^{d} x_{ij} b_j$ then

$$\frac{\partial f}{\partial x_{ij}} = a_i b_j \quad \Longrightarrow \quad \frac{\partial f}{\partial X} = \begin{pmatrix} a_1 b_1 & a_1 b_2 & \ldots & a_1 b_d \\ \vdots & \vdots & \vdots & \vdots \\ a_d b_1 & a_d b_2 & \ldots & a_d b_d \end{pmatrix} = \mathbf{a}\mathbf{b}^T$$



**Derivative of a linear function**

$$\frac{\partial \mathbf{x}^T\mathbf{a}}{\partial \mathbf{x}} = \mathbf{a} \quad (1)$$

$$\frac{\partial \mathbf{a}^T\mathbf{x}}{\partial \mathbf{x}} = \mathbf{a} \quad (2)$$

$$\frac{\partial \mathbf{a}^T X \mathbf{b}}{\partial X} = \mathbf{a}\mathbf{b}^T \quad (3)$$

$$\frac{\partial \mathbf{a}^T X^T \mathbf{b}}{\partial X} = \mathbf{b}\mathbf{a}^T \quad (4)$$

## Matrix Calculus

**Derivative of a quadratic function**

$$\frac{\partial \mathbf{x}^T B \mathbf{x}}{\partial \mathbf{x}} = (B + B^T)\mathbf{x} \tag{5}$$

$$\frac{\partial \mathbf{b}^T X^T X \mathbf{c}}{\partial X} = X(\mathbf{b}\mathbf{c}^T + \mathbf{c}\mathbf{b}^T) \tag{6}$$

$$\frac{\partial (B\mathbf{x} + \mathbf{b})^T C (D\mathbf{x} + \mathbf{d})}{\partial \mathbf{x}} = B^T C (D\mathbf{x} + \mathbf{d}) + D^T C^T (B\mathbf{x} + \mathbf{b}) \tag{7}$$

$$\frac{\partial \mathbf{b}^T X^T D X \mathbf{c}}{\partial X} = D^T X \mathbf{b}\mathbf{c}^T + D X \mathbf{c}\mathbf{b}^T \tag{8}$$

**End of Technical interlude**

## Pseudo-Inverse solution

- Can write the cost function as

$$L(\mathcal{D}, \mathbf{w}, b) = \frac{1}{2} \sum_{(\mathbf{x},y)\in\mathcal{D}} \left(\mathbf{w}^T\mathbf{x} + b - y\right)^2 = \frac{1}{2} \sum_{(\mathbf{x},y)\in\mathcal{D}} \left(\mathbf{w}_1^T\mathbf{x}' - y\right)^2$$

  where $\mathbf{x}' = (\mathbf{x}^T, 1)^T, \mathbf{w}_1 = (\mathbf{w}^T, b)^T$

- Writing in matrix notation this becomes

$$\begin{aligned} L(\mathcal{D}, \mathbf{w}_1) = \frac{1}{2}\|X\mathbf{w}_1 - \mathbf{y}\|^2 &= \frac{1}{2}(X\mathbf{w}_1 - \mathbf{y})^T(X\mathbf{w}_1 - \mathbf{y}) \\ &= \frac{1}{2}\left(\mathbf{w}_1^T X^T X \mathbf{w}_1 - 2\mathbf{y}^T X \mathbf{w}_1 + \mathbf{y}^T\mathbf{y}\right) \end{aligned}$$

  where

$$\mathbf{y} = (y_1, \ldots, y_n)^T, \quad \mathbf{w} = (w_1, \ldots, w_{d+1})^T, \quad X = \begin{pmatrix} \mathbf{x}_1^T & 1 \\ \vdots & \vdots \\ \mathbf{x}_n^T & 1 \end{pmatrix}$$

## Pseudo-Inverse solution

- The gradient of $L(\mathcal{D}, \mathbf{w}_1)$ w.r.t. $\mathbf{w}_1$:

$$\nabla_{\mathbf{w}_1} L(\mathcal{D}, \mathbf{w}_1) = X^T X \mathbf{w}_1 - X^T \mathbf{y}$$

- Setting this equal to zero yields $X^T X \mathbf{w}_1 = X^T \mathbf{y}$ and

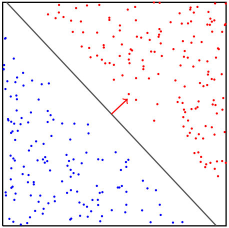
$$\mathbf{w}_1 = X^\dagger \mathbf{y}$$

  where

$$X^\dagger \equiv \left(X^T X\right)^{-1} X^T$$

- $X^\dagger$ is called the **pseudo-inverse** of $X$. Note that $X^\dagger X = I$ but in general $X X^\dagger \neq I$.

## Simple 2D Example



Decision boundary found by minimizing

$$L_{\text{squared error}}(\mathcal{D}, \mathbf{w}, b) = \sum_{(\mathbf{x},y)\in\mathcal{D}} \left(y - (\mathbf{w}^T\mathbf{x} + b)\right)^2$$

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- $X^\dagger$ is called the **pseudo-inverse** of $X$. Note that $X^\dagger X = I$ but in general $X X^\dagger \neq I$.
- If $X^T X$ singular $\implies$ no unique solution to $X^T X \mathbf{w} = X^T \mathbf{y}$.

## Technical interlude: Iterative Optimization

## Iterative Optimization

- Common approach to solving such unconstrained optimization problem is iterative non-linear optimization.

$$\mathbf{x}^* = \arg\min_{\forall \mathbf{x}} f(\mathbf{x})$$

- Start with an estimate $\mathbf{x}^{(0)}$.
- Try to improve it by finding successive new estimates $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \ldots$ s.t. $f(\mathbf{x}^{(1)}) \geq f(\mathbf{x}^{(2)}) \geq f(\mathbf{x}^{(3)}) \geq \cdots$ until convergence.
- To find a better estimate at each iteration: Perform the search locally around the current estimate.
- Such iterative approaches will find a local minima.

## Iterative Optimization

Iterative optimization methods alternate between these two steps:

**Decide search direction**

Choose a search direction based on the local properties of the cost function.

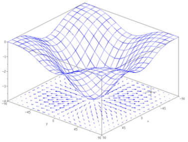
**Line Search**

Perform an intensive search to find the minimum along the chosen direction.

## Choosing a search direction: The gradient

The gradient is defined as:

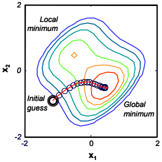
$$\nabla_{\mathbf{x}} f(\mathbf{x}) \equiv \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_d} \end{pmatrix}$$



The gradient points in the direction of the greatest increase of $f(\mathbf{x})$.

## Gradient descent: Method for function minimization

Gradient descent finds the minimum in an iterative fashion by moving in the direction of steepest descent.




**Gradient Descent Minimization**

1. Start with an arbitrary solution $\mathbf{x}^{(0)}$.
2. Compute the gradient $\nabla_{\mathbf{x}} f(\mathbf{x}^{(k)})$.
3. Move in the direction of steepest descent:

   $$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \eta^{(k)} \nabla_{\mathbf{x}} f(\mathbf{x}^{(k)}).$$

   where $\eta^{(k)}$ is the step size.
4. Go to 2 (until convergence).

## Gradient descent: Method for function minimization

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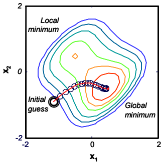


**Gradient Descent Minimization**

**Properties**

1. Will converge to a local minimum.
2. The local minimum found depends on the initialization $\mathbf{x}^{(0)}$.

**But this is okay**

1. For convex optimization problems: **local minimum** $\equiv$ **global minimum**
2. For deep networks most parameter setting corresponding to a **local minimum** are fine.

## Gradient descent: Method for function minimization

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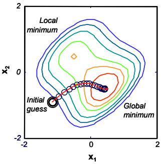


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**End of Technical interlude**

## Gradient descent solution

The error function $L(\mathcal{D}, \mathbf{w}_1)$ could also be minimized wrt $\mathbf{w}_1$ by using a **gradient descent procedure**.

**Why?**

- This avoids the numerical problems that arise when $X^T X$ is (nearly) singular.
- It also avoids the need for working with large matrices.

**How**

1. Begin with an initial guess $\mathbf{w}_1^{(0)}$ for $\mathbf{w}_1$.
2. Update the weight vector by moving a small distance in the direction $-\nabla_{\mathbf{w}_1} L$.

## Gradient descent solution

**Solution**

$$\mathbf{w}_1^{(t+1)} = \mathbf{w}_1^{(t)} - \eta^{(t)} X^T (X \mathbf{w}_1^{(t)} - \mathbf{y})$$

- If $\eta^{(t)} = \eta_0 / t$, where $\eta_0 > 0$, then
- $\mathbf{w}_1^{(0)}, \mathbf{w}_1^{(1)}, \mathbf{w}_1^{(2)}, \ldots$ converges to a solution of

$$X^T (X \mathbf{w}_1 - \mathbf{y}) = \mathbf{0}$$

- Irrespective of whether $X^T X$ is singular or not.

## Stochastic gradient descent solution

- Increase the number of updates per computation by considering each training sample sequentially

$$\mathbf{w}_1^{(t+1)} = \mathbf{w}_1^{(t)} - \eta^{(t)}(\mathbf{x}_i^T \mathbf{w}_1^{(t)} - y_i)\mathbf{x}_i$$

- This is known as the **Widrow-Hoff**, **least-mean-squares** (LMS) or **delta rule** [Mitchell, 1997].

- More generally this is an application of **Stochastic Gradient Descent**.

## Technical interlude: Stochastic Gradient Descent

## Common Optimization Problem in Machine Learning

- **Form of the optimization problem**:

$$J(\mathcal{D}, \boldsymbol{\theta}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x}, y) \in \mathcal{D}} l(y, f(\mathbf{x}; \boldsymbol{\theta})) + \lambda R(\boldsymbol{\theta})$$

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} J(\mathcal{D}, \boldsymbol{\theta})$$

- **Solution with gradient descent**
  1. Start with a random guess $\boldsymbol{\theta}^{(0)}$ for the parameters.
  2. Then iterate until convergence

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta^{(t)} \nabla_{\boldsymbol{\theta}} J(\mathcal{D}, \boldsymbol{\theta})|_{\boldsymbol{\theta}^{(t)}}$$

## Given large scale data

If $|\mathcal{D}|$ is large

- $\Longrightarrow$ computing $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}, \mathcal{D})|_{\boldsymbol{\theta}^{(t)}}$ is time consuming
- $\Longrightarrow$ each update of $\boldsymbol{\theta}^{(t)}$ takes lots of computations
- Gradient descent needs lots of iterations to converge as $\eta$ usually small
- $\Longrightarrow$ GD takes an age to find a local optimum.

## Work around: Stochastic Gradient Descent

- Start with a random solution $\boldsymbol{\theta}^{(0)}$.
- Until convergence for $t = 1, \ldots$
  1. Randomly select $(\mathbf{x}, y) \in \mathcal{D}$.
  2. Set $\mathcal{D}^{(t)} = \{(\mathbf{x}, y)\}$.
  3. Update parameter estimate with

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta^{(t)} \, \nabla_{\boldsymbol{\theta}} J(\mathcal{D}^{(t)}, \boldsymbol{\theta})\Big|_{\boldsymbol{\theta}^{(t)}}$$

## Comments about SGD

- When $|\mathcal{D}^{(t)}| = 1$:

  $\nabla_{\boldsymbol{\theta}} J(\mathcal{D}^{(t)}, \boldsymbol{\theta})\big|_{\boldsymbol{\theta}^{(t)}}$ a noisy estimate of $\nabla_{\boldsymbol{\theta}} J(\mathcal{D}, \boldsymbol{\theta})\big|_{\boldsymbol{\theta}^{(t)}}$
- Therefore

  $|\mathcal{D}|$ **noisy** update steps in SGD $\approx$ 1 **correct** update step in GD.
- In practice SGD converges a lot faster then GD.
- Given lots of labelled training data:

  **Quantity** of updates more important than **quality** of updates!

## Best practices for SGD

- **Preparing the data**
  - Randomly shuffle the training examples and zip sequentially through $\mathcal{D}$.
  - Use preconditioning techniques.
- **Monitoring and debugging**
  - Monitor both the training cost and the validation error.
  - Check the gradients using finite differences.
  - Experiment with learning rates $\eta^{(t)}$ using a small sample of the training set.

## Mini-Batch Gradient Descent

- Start with a random guess $\boldsymbol{\theta}^{(0)}$ for the parameters.
- Until convergence for $t = 1, \ldots$
  1. Randomly select a subset $\mathcal{D}^{(t)} \subset \mathcal{D}$ s.t. $|\mathcal{D}^{(t)}| = n_b$ (typically $n_b \approx 150$.)
  2. Update parameter estimate with

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta^{(t)} \, \nabla_{\boldsymbol{\theta}} J(\mathcal{D}^{(t)}, \boldsymbol{\theta})\Big|_{\boldsymbol{\theta}^{(t)}}$$

## Benefits of mini-batch gradient descent

- Obtain a more accurate estimate of $\nabla_{\boldsymbol{\theta}} J(\mathcal{D}, \boldsymbol{\theta})|_{\boldsymbol{\theta}^{(t)}}$ than in SGD.
- Still get lots of updates per epoch (one iteration through all the training data).

**End of Technical interlude**

## What learning rate?

- **Issues with setting the learning rate $\eta^{(t)}$?**
  - Larger $\eta$'s $\Longrightarrow$ potentially faster learning but with the risk of less stable convergence.
  - Smaller $\eta$'s $\Longrightarrow$ slow learning but stable convergence.
- **Strategies**
  - Constant: $\eta^{(t)} = .01$
  - Decreasing: $\eta^{(t)} = 1/\sqrt{t}$
- **Lots of recent algorithms dealing with this issue**

  Will describe these algorithms in the near future.

**Squared Error loss + $L_2$ regularization**

## Add an $L_2$ regularization term (a.k.a. ridge regression)

- Add a regularization term to the loss function

$$J_{\text{ridge}}(\mathcal{D}, \mathbf{w}, b) = \frac{1}{2} \sum_{(\mathbf{x}, y) \in \mathcal{D}} l_{\text{sq}}(y, \mathbf{w}^T \mathbf{x} + b) + \lambda \|\mathbf{w}\|^2$$

$$= \frac{1}{2} \|X\mathbf{w} + b\mathbf{1} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$$

where $\lambda > 0$ and small and $X$ is the data matrix

$$X = \begin{pmatrix} \leftarrow & \mathbf{x}_1^T & \rightarrow \\ \leftarrow & \mathbf{x}_2^T & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^T & \rightarrow \end{pmatrix}$$

## Solving Ridge Regression: Centre the data to simplify

- Add a regularization term to the loss function

$$J_{\text{ridge}}(\mathcal{D}, \mathbf{w}, b) = \frac{1}{2} \|X\mathbf{w} + b\mathbf{1} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$$

- Let's centre the input data

$$X_c = \begin{pmatrix} \leftarrow & \mathbf{x}_{c,1}^T & \rightarrow \\ \leftarrow & \mathbf{x}_{c,2}^T & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_{c,n}^T & \rightarrow \end{pmatrix} \quad \text{where } \mathbf{x}_{c,i} = \mathbf{x}_i - \boldsymbol{\mu}_{\mathbf{x}}$$

$$\implies X_c^T \mathbf{1} = \mathbf{0}.$$

- Optimal bias with centered input $X_c$ (does not depend on $\mathbf{w}^*$) is:

$$\frac{\partial J_{\text{ridge}}}{\partial b} = b\mathbf{1}^T\mathbf{1} + \mathbf{w}^T X_c^T \mathbf{1} - \mathbf{1}^T \mathbf{y}$$

$$= b\mathbf{1}^T\mathbf{1} - \mathbf{1}^T \mathbf{y}$$

$$\implies b^* = 1/n \sum_{i=1}^n y_i = \bar{y}.$$

## Solving ridge regression: Optimal weight vector

- Add a regularization term to the loss function

$$J_{\text{ridge}}(\mathcal{D}, \mathbf{w}) = \frac{1}{2} \|X_c\mathbf{w} + \bar{y}\mathbf{1} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$$

- Compute the gradient of $J_{\text{ridge}}$ w.r.t. $\mathbf{w}$

$$\frac{\partial J_{\text{ridge}}}{\partial \mathbf{w}} = \left(X_c^T X_c + \lambda I_d\right) \mathbf{w} - X_c^T \mathbf{y}$$

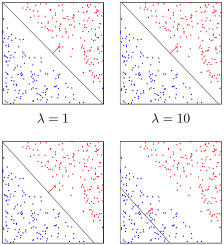
- Set to zero to get

$$\mathbf{w}^* = \left(X_c^T X_c + \lambda I_d\right)^{-1} X_c^T \mathbf{y}$$

- $(X_c^T X_c + \lambda I_d)$ has a unique inverse even if $X_c^T X_c$ is singular.

## Simple 2D Example

Ridge Regression decision boundaries as $\lambda$ is varied



$\lambda = 1$ $\lambda = 10$

$\lambda = 100$ $\lambda = 1000$

## Solving ridge regression: Optimal weight vector

- Add a regularization term to the loss function

$$J_{\text{ridge}}(\mathcal{D}, \mathbf{w}) = \frac{1}{2}\|X_c\mathbf{w} + \bar{y}\mathbf{1} - \mathbf{y}\|^2 + \lambda\|\mathbf{w}\|^2$$

- Compute the gradient of $J_{\text{ridge}}$ w.r.t. $\mathbf{w}$

$$\frac{\partial J_{\text{ridge}}}{\partial \mathbf{w}} = \left(X_c^T X_c + \lambda I_d\right)\mathbf{w} - X_c^T\mathbf{y}$$

- Set to zero to get

$$\mathbf{w}^* = \left(X_c^T X_c + \lambda I_d\right)^{-1} X_c^T\mathbf{y}$$

- $(X_c^T X_c + \lambda I_d)$ has a unique inverse even if $X_c^T X_c$ is singular.

- If $d$ is large $\implies$ have to invert a very large matrix.

## Solving ridge regression: Iteratively

- The gradient-descent update step is

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta\left[\left(X_c^T X_c + \lambda I_d\right)\mathbf{w}^{(t)} - X_c^T\mathbf{y}\right]$$

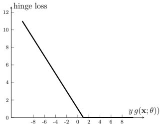
- The SGD update step for sample $(\mathbf{x}, y)$ is

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta\left[\left((\mathbf{x} - \boldsymbol{\mu}_x)(\mathbf{x} - \boldsymbol{\mu}_x)^T + \lambda I_d\right)\mathbf{w}^{(t)} - (\mathbf{x} - \boldsymbol{\mu}_x)y\right]$$

## Hinge Loss

## The Hinge loss

$$l(\mathbf{x}, y; \mathbf{w}, b) = \max\left\{0, 1 - y(\mathbf{w}^T\mathbf{x} + b)\right\}$$




- This loss is not differentiable but is convex.

- Correctly classified examples *sufficiently* far from the decision boundary have zero loss.

- $\implies$ have a way of choosing between classifiers that correctly classify all the training examples.

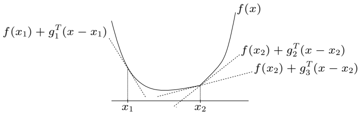
## Technical interlude: Sub-gradient



- $\mathbf{g}$ is a **subgradient** of $f$ at $\mathbf{x}$ if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^T(\mathbf{y} - \mathbf{x}) \quad \forall \mathbf{y}$$

- **1D example**:

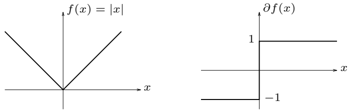



  - $g_2, g_3$ are subgradients at $x_2$;
  - $g_1$ is a subgradient at $x_1$.



- Set of all subgradients of $f$ at $\mathbf{x}$ is called the subdifferential of $f$ at $\mathbf{x}$, written $\partial f(\mathbf{x})$

- **1D example**:




- If $f$ is convex and differentiable: $\nabla f(\mathbf{x})$ a subgradient of $f$ at $\mathbf{x}$.

## End of Technical interlude

## The Hinge loss

- Find $\mathbf{w}, b$ that minimize

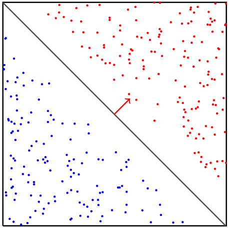
$$L_{\text{hinge}}(\mathcal{D}, \mathbf{w}, b) = \sum_{(\mathbf{x},y)\in\mathcal{D}} \underbrace{\max\left\{0, 1 - y(\mathbf{w}^T\mathbf{x} + b)\right\}}_{\text{Hinge Loss}}$$

- Can use stochastic gradient descent to do the optimization.
- The (sub-)gradients of the hinge-loss are

$$\nabla_{\mathbf{w}} l(\mathbf{x}, y; \mathbf{w}, b) = \begin{cases} -y\,\mathbf{x} & \text{if } y(\mathbf{w}^T\mathbf{x} + b) < 1 \\ 0 & \text{otherwise.} \end{cases}$$

$$\frac{\partial\, l(\mathbf{x}, y; \mathbf{w}, b)}{\partial b} = \begin{cases} -y & \text{if } y(\mathbf{w}^T\mathbf{x} + b) < 1 \\ 0 & \text{otherwise.} \end{cases}$$

## Example of decision boundary found



Decision boundary found by minimizing with SGD

$$L_{\text{hinge}}(\mathcal{D}, \mathbf{w}, b) = \sum_{(\mathbf{x},y)\in\mathcal{D}} \max\left\{0, 1 - y(\mathbf{w}^T\mathbf{x} + b)\right\}$$

**$L_2$ Regularization + Hinge Loss**

## $L_2$ regularization + Hinge loss

- Find $\mathbf{w}, b$ that minimize

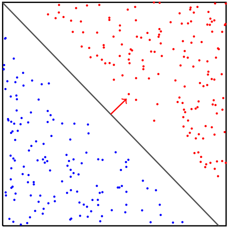
$$J_{\text{svm}}(\mathcal{D}, \mathbf{w}, b) = \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{(\mathbf{x},y)\in\mathcal{D}} \underbrace{\max\left\{0, 1 - y(\mathbf{w}^T\mathbf{x} + b)\right\}}_{\text{Hinge Loss}}$$

- Can use stochastic gradient descent to do the optimization.
- The sub-gradients of this cost function

$$\nabla_{\mathbf{w}} l(\mathbf{x}, y; \mathbf{w}, b) = \begin{cases} \lambda\mathbf{w} - y\,\mathbf{x} & \text{if } y(\mathbf{w}^T\mathbf{x} + b) < 1 \\ \lambda\mathbf{w} & \text{otherwise.} \end{cases}$$

$$\frac{\partial\, l(\mathbf{x}, y; \mathbf{w}, b)}{\partial b} = \begin{cases} -y & \text{if } y(\mathbf{w}^T\mathbf{x} + b) < 1 \\ 0 & \text{otherwise.} \end{cases}$$

## Example of decision boundary found



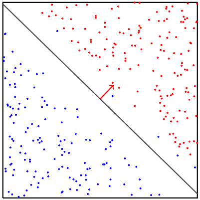
Decision boundary found with SGD by minimizing ($\lambda = .01$)

$$J_{\text{hinge}}(\mathcal{D}, \mathbf{w}, b) = \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{(\mathbf{x},y)\in\mathcal{D}} \max\left\{0, 1 - y(\mathbf{w}^T\mathbf{x} + b)\right\}$$

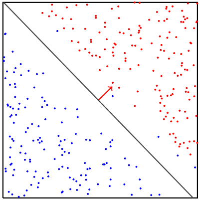
**"$L_2$ Regularization + Hinge Loss" $\equiv$ SVM**

## Regularization reduces the influence of *outliers*

Decision boundaries found by minimizing



**Hinge Loss**



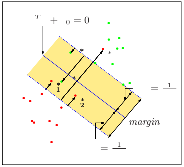
$L_2$ **Regularization + Hinge Loss**

## SVM's constrained optimization problem

SVM solves this constrained optimization problem:

$$\min_{\mathbf{w},b}\left(\frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{n}\xi_i\right) \quad \textbf{subject to}$$

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i \ \text{ for } i = 1, \ldots, n \quad \textbf{and}$$
$$\xi_i \geq 0 \ \text{ for } i = 1, \ldots, n.$$



## Alternative formulation of SVM optimization

SVM solves this constrained optimization problem:

$$\min_{\mathbf{w},b} \left( \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{n} \xi_i \right) \quad \textbf{subject to}$$

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i \;\text{ for } i = 1, \ldots, n \quad \textbf{and}$$
$$\xi_i \geq 0 \;\text{ for } i = 1, \ldots, n.$$

- Let's look at the constraints:

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i \quad \Longrightarrow \quad \xi_i \geq 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)$$

- But $\xi_i \geq 0$ also, therefore

$$\boxed{\xi_i \;\geq\; \max\left\{0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right\}}$$

## Alternative formulation of the SVM optimization

Thus the original constrained optimization problem can be restated as an **unconstrained optimization problem**:

$$\min_{\mathbf{w},b} \left( \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\textbf{Regularization term}} + C\sum_{i=1}^{n} \underbrace{\max\left\{0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right\}}_{\textbf{Hinge loss}} \right)$$

and corresponds to the $L_2$ **regularization + Hinge loss** formulation!

$\Longrightarrow$ can train SVMs with SGD/mini-batch gradient descent.

## Alternative formulation of the SVM optimization

Thus the original constrained optimization problem can be restated as an **unconstrained optimization problem**:

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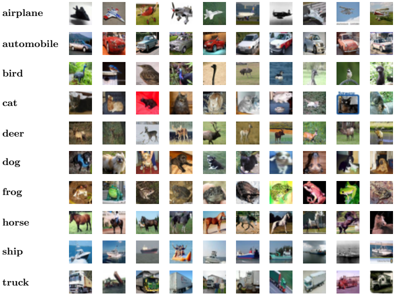
and corresponds to the $L_2$ **regularization + Hinge loss** formulation!

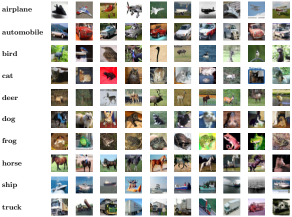
$\Longrightarrow$ can train SVMs with SGD/mini-batch gradient descent.

## From binary to multi-class classification

## Example dataset: CIFAR-10




## Example dataset: CIFAR-10




**CIFAR-10**

- 10 classes
- 50,000 training images
- 10,000 test images
- Each image has size $32 \times 32 \times 3$

## Technical description of the multi-class problem

- Have a set of labelled training examples

  $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ with each $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \{1, \ldots, C\}$.

- Want to learn from $\mathcal{D}$ a classification function

$$g : \underset{\text{input space}}{\underset{\uparrow}{\mathbb{R}^d}} \times \underset{\text{parameter space}}{\underset{\uparrow}{\mathbb{R}^P}} \rightarrow \{1, \ldots, C\}$$

  Usually

$$g(\mathbf{x}; \boldsymbol{\Theta}) = \arg \max_{1 \leq j \leq C} f_j(\mathbf{x}; \boldsymbol{\theta}_j)$$

  where for $j = 1, \ldots, C$:

$$f_j : \mathbb{R}^d \times \mathbb{R}^p \rightarrow \mathbb{R}$$

  and $\boldsymbol{\Theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_C)$.

## Multi-class linear classifier

- Let each $f_j$ be a linear function that is

$$f_j(\mathbf{x}; \boldsymbol{\theta}_j) = \mathbf{w}_j^T \mathbf{x} + b_j$$

- Define

$$f(\mathbf{x}; \boldsymbol{\Theta}) = \begin{pmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_C(\mathbf{x}) \end{pmatrix}$$

  then

$$f(\mathbf{x}; \boldsymbol{\Theta}) = f(\mathbf{x}; W, \mathbf{b}) = W\mathbf{x} + \mathbf{b}$$

  where

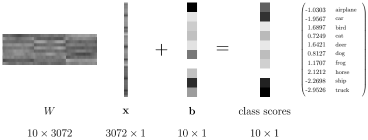
$$W = \begin{pmatrix} \mathbf{w}_1^T \\ \vdots \\ \mathbf{w}_C^T \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_C \end{pmatrix}$$

- Note $W$ has size $C \times d$ and $\mathbf{b}$ is $C \times 1$.

## Apply a multi-class linear classifier to an image

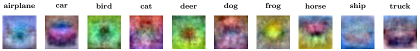
- Have a 2D colour image but can flatten it into a 1D vector $\mathbf{x}$


- Apply classifier: $W\mathbf{x} + \mathbf{b}$ to get a score for each class.



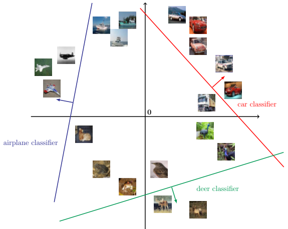

## Interpreting a multi-class linear classifier

- Learn $W, \mathbf{b}$ to classify the images in a dataset.
- Can interpret each row, $\mathbf{w}_j$, of $W$ as a template for class $j$.
- Below is the visualization of each learnt $\mathbf{w}_j$ for CIFAR-10




## Interpreting a multi-class linear classifier

- Each $\mathbf{w}_j^T\mathbf{x} + b_j = 0$ corresponds to a hyperplane, $H_j$, in $\mathbb{R}^d$.
- $\text{sign}(\mathbf{w}_j^T\mathbf{x} + b_j)$ tells us which side of $H_j$ the point $\mathbf{x}$ lies.
- The score $|\mathbf{w}_j^T\mathbf{x} + b_j| \propto$ the distance of $\mathbf{x}$ to $H_j$.




## How do we learn $W$ and $\mathbf{b}$?

As before need to

- Specify a loss function (+ a regularization term).
- Set up the optimization problem.
- Perform the optimization.

## How do we learn $W$ and $\mathrm{b}$?

As before need to

- Specify a loss function
  - must quantify the quality of all the class scores across all the training data.
- Set up the optimization problem.
- Perform the optimization.

## Multi-class loss functions

## Multi-class SVM Loss

- Remember have training data

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \quad \text{with each } \mathbf{x}_i \in \mathbb{R}^d,\ y_i \in \{1, \ldots, C\}.$$

- Let $s_j$ be the score of function $f_j$ applied to $\mathbf{x}$

$$s_j = f_j(\mathbf{x}; \mathbf{w}_j, b_j) = \mathbf{w}_j^T \mathbf{x} + b_j$$

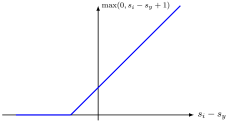
- The SVM loss for training example $\mathbf{x}$ with label $y$ is

$$l = \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, s_j - s_y + 1)$$

## Multi-class SVM Loss

- $s_j$ is the score of function $f_j$ applied to $\mathbf{x}$

$$s_j = f_j(\mathbf{x}; \mathbf{w}_j, b_j) = \mathbf{w}_j^T \mathbf{x} + b_j$$




- SVM loss for training example $\mathbf{x}$ with label $y$ is

$$l = \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, s_j - s_y + 1)$$

## Calculate the multi-class SVM loss for a CIFAR image

| input: $\mathbf{x}$ | output | label | loss |
|---|---|---|---|
|  | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $y = 8$ | $l = \sum_{\substack{j=1 \\ j \neq y}}^{10} \max(0, s_j - s_y + 1)$ |

| | Scores |
|---|---|
| airplane | -0.3166 |
| car | -0.6609 |
| bird | 0.7058 |
| cat | 0.8538 |
| deer | 0.6525 |
| dog | 0.1874 |
| frog | 0.6072 |
| horse | 0.5134 |
| ship | -1.3490 |
| truck | -1.2225 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ |

## Calculate the multi-class SVM loss for a CIFAR image

| input: $\mathbf{x}$ | output | label | loss |
|---|---|---|---|
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| | Scores | Compare to horse score |
|---|---|---|
| airplane | -0.3166 | 0.1701 |
| car | -0.6609 | -0.1743 |
| bird | 0.7058 | 1.1925 |
| cat | 0.8538 | 1.3405 |
| deer | 0.6525 | 1.1392 |
| dog | 0.1874 | 0.6741 |
| frog | 0.6072 | 1.0938 |
| horse | 0.5134 | 1.0000 |
| ship | -1.3490 | -0.8624 |
| truck | -1.2225 | -0.7359 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $\mathbf{s} - s_8 + 1$ |

## Calculate the multi-class SVM loss for a CIFAR image

| input: $\mathbf{x}$ | output | label | loss |
|---|---|---|---|
|  | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $y = 8$ | $l = \sum_{\substack{j=1 \\ j \neq y}}^{10} \max(0, s_j - s_y + 1)$ |

| | Scores | Compare to horse score | Keep badly performing classes |
|---|---|---|---|
| airplane | -0.3166 | 0.1701 | 0.1701 |
| car | -0.6609 | -0.1743 | 0 |
| bird | 0.7058 | 1.1925 | 1.1925 |
| cat | 0.8538 | 1.3405 | 1.3405 |
| deer | 0.6525 | 1.1392 | 1.1392 |
| dog | 0.1874 | 0.6741 | 0.6741 |
| frog | 0.6072 | 1.0938 | 1.0938 |
| horse | 0.5134 | 1.0000 | 1.0000 |
| ship | -1.3490 | -0.8624 | 0 |
| truck | -1.2225 | -0.7359 | 0 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $\mathbf{s} - s_8 + 1$ | $\max(0, \mathbf{s} - s_8 + 1)$ |

**Loss** for $\mathbf{x}$: 5.4723

## Problem with the SVM loss

Given $W$ and $\mathbf{b}$ then

- Response for one training example

$$f(\mathbf{x}; W, \mathbf{b}) = W\mathbf{x} + \mathbf{b} = \mathbf{s}$$

- **loss for $\mathbf{x}$**

$$l(\mathbf{x}, y, W, \mathbf{x}) = \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, s_j - s_y + 1)$$

- **Loss over all the training data**

$$L(\mathcal{D}, W, \mathbf{b}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y) \in \mathcal{D}} l(\mathbf{x}, y, W, \mathbf{b})$$

Have found a $W$ s.t. $L = 0$. Is this $W$ unique?

Let $W_1 = \alpha W$ and $\mathbf{b}_1 = \alpha \mathbf{b}$ where $\alpha > 1$ then

- Response for one training example

$$f(\mathbf{x}; W_1, \mathbf{b}) = W_1 \mathbf{x} + \mathbf{b}_1 = \mathbf{s}' = \alpha(W\mathbf{x} + \mathbf{b})$$

- **Loss for** $(\mathbf{x}, y)$ w.r.t. $W_1$ and $\mathbf{b}_1$

$$\begin{aligned} l(\mathbf{x}, y, W_1, \mathbf{b}_1) &= \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, s'_j - s'_y + 1) \\ &= \max(0, \alpha(\mathbf{w}_j^T \mathbf{x} + b_j - \mathbf{w}_y^T \mathbf{x} - b_y) + 1) \\ &= \max(0, \alpha(s_j - s_y) + 1) \\ &= 0 \quad \text{as by definition } s_j - s_y < -1 \text{ and } \alpha > 1 \end{aligned}$$

- Thus the total loss $L(\mathcal{D}, W_1, \mathbf{b}_1)$ is 0.

## Cross-entropy Loss



$$L(\mathcal{D}, W, \mathbf{b}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, f_j(\mathbf{x}; W, \mathbf{b}) - f_y(\mathbf{x}; W, \mathbf{b}) + 1) + \lambda R(W)$$

**Commonly used Regularization**

| Name of regularization | Mathematical def. of $R(W)$ |
|---|---|
| $L_2$ | $\sum_k \sum_l W_{k,l}^2$ |
| $L_1$ | $\sum_k \sum_l \lvert W_{k,l}\rvert$ |
| Elastic Net | $\sum_k \sum_l \left(\beta W_{k,l}^2 + \lvert W_{k,l}\rvert\right)$ |

## Probabilistic interpretation of scores

Let $p_j$ be the probability that input $\mathbf{x}$ has label $j$:

$$P_{Y|\mathbf{X}}(j \mid \mathbf{x}) = p_j$$

- For $\mathbf{x}$ our linear classifier outputs scores for each class:

$$\mathbf{s} = W\mathbf{x} + \mathbf{b}$$

- Can interpret scores, $\mathbf{s}$, as:

  **unnormalized log probability for each class**.

  $\Longrightarrow$

$$s_j = \log p'_j$$

  where $\alpha p'_j = p_j$ and $\alpha = \sum p'_j$.

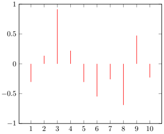
  $\Longrightarrow$

$$P_{Y|\mathbf{X}}(j \mid \mathbf{x}) = p_j = \frac{\exp(s_j)}{\sum_k \exp(s_k)}$$

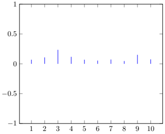
## Softmax operation

- This transformation is known as

$$\text{Softmax}(\mathbf{s}) = \frac{\exp(s_j)}{\sum_k \exp(s_k)}$$




$\mathbf{x}$




Softmax($\mathbf{x}$)

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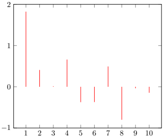
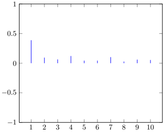
$$\text{Softmax}(\mathbf{s}) = \frac{\exp(s_j)}{\sum_k \exp(s_k)}$$




$\mathbf{x}$




Softmax($\mathbf{x}$)

## Softmax classifier: Log likelihood of the training data

- **Given probabilistic model**: Estimate its parameters by maximizing the log-likelihood of the training data.

$$\begin{aligned}\boldsymbol{\theta}^* &= \arg\max_{\boldsymbol{\theta}} \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \log P_{Y|\mathbf{X}}(y \mid \mathbf{x}; \boldsymbol{\theta}) \\ &= \arg\min_{\boldsymbol{\theta}} \; -\frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \log P_{Y|\mathbf{X}}(y \mid \mathbf{x}; \boldsymbol{\theta})\end{aligned}$$

- Given probabilistic interpretation of our classifier, the negative log-likelihood of the training data is

$$-\frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \log \left( \frac{\exp(s_y)}{\sum_{k=1}^{C} \exp(s_k)} \right)$$

where $\mathbf{s} = W\mathbf{x} + \mathbf{b}$.

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## Softmax classifier + cross-entropy loss

- Given the probabilistic interpretation of our classifier, the negative log-likelihood of the training data is

$$L(\mathcal{D}, W, \mathbf{b}) = -\frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \log\left(\frac{\exp(s_y)}{\sum_{k=1}^{C}\exp(s_k)}\right)$$

where $\mathbf{s} = W\mathbf{x} + \mathbf{b}$.

- Can also interpret this in terms of the cross-entropy loss:

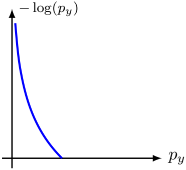
$$L(\mathcal{D}, W, \mathbf{b}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} \underbrace{-\log\left(\frac{\exp(s_y)}{\sum_{k=1}^{C}\exp(s_k)}\right)}_{\text{cross-entropy loss for } (\mathbf{x}, y)}$$

$$= \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} l(\mathbf{x}, y, W, \mathbf{b})$$

## Cross-entropy loss

- $\mathbf{p}$ the probability vector the *network* assigns to $\mathbf{x}$ for each class

$$\mathbf{p} = \text{SOFTMAX}\,(W\mathbf{x} + \mathbf{b})$$




- Cross-entropy loss for training example $\mathbf{x}$ with label $y$ is

$$l = -\log(p_y)$$

## Calculate the cross-entropy loss for a CIFAR image

| input: $\mathbf{x}$ | output | label | loss |
|---|---|---|---|
|  | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $y = 8$ | $l = -\log\left(\frac{\exp(s_y)}{\sum\exp(s_k)}\right)$ |

| | Scores |
|---|---|
| airplane | -0.3166 |
| car | -0.6609 |
| bird | 0.7058 |
| cat | 0.8538 |
| deer | 0.6525 |
| dog | 0.1874 |
| frog | 0.6072 |
| horse | 0.5134 |
| ship | -1.3490 |
| truck | -1.2225 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ |

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| | Scores | exp(Scores) |
|---|---|---|
| airplane | -0.3166 | 0.7354 |
| car | -0.6609 | 0.5328 |
| bird | 0.7058 | 2.0203 |
| cat | 0.8538 | 2.3583 |
| deer | 0.6525 | 1.9303 |
| dog | 0.1874 | 1.2080 |
| frog | 0.6072 | 1.8319 |
| horse | 0.5134 | 1.7141 |
| ship | -1.3490 | 0.2585 |
| truck | -1.2225 | 0.2945 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $\exp(\mathbf{s})$ |

input: $\mathbf{x}$ | output | label | loss

$\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $y = 8$ | $l = -\log\left(\frac{\exp(s_y)}{\sum \exp(s_k)}\right)$

| | Scores | exp(Scores) | Normalized scores |
|---|---|---|---|
| airplane | -0.3166 | 0.7354 | 0.0571 |
| car | -0.6609 | 0.5328 | 0.0414 |
| bird | 0.7058 | 2.0203 | 0.1568 |
| cat | 0.8538 | 2.3583 | 0.1830 |
| deer | 0.6525 | 1.9303 | 0.1498 |
| dog | 0.1874 | 1.2080 | 0.0938 |
| frog | 0.6072 | 1.8319 | 0.1422 |
| horse | 0.5134 | 1.7141 | 0.1330 |
| ship | -1.3490 | 0.2585 | 0.0201 |
| truck | -1.2225 | 0.2945 | 0.0229 |
| | $\mathbf{s} = W\mathbf{x} + \mathbf{b}$ | $\exp(\mathbf{s})$ | $\frac{\exp(\mathbf{s})}{\sum_k \exp(s_k)}$ |

**Loss** for $\mathbf{x}$: 2.0171



**Cross-entropy loss**

$$l(\mathbf{x}, y, W, \mathbf{b}) = -\log\left(\frac{\exp(s_y)}{\sum_{k=1}^{C} \exp(s_k)}\right)$$

**Questions**

- What is the minimum possible value of $l(\mathbf{x}, y, W, \mathbf{b})$?
- What is the max possible value of $l(\mathbf{x}, y, W, \mathbf{b})$?
- At initialization all the entries of $W$ are small $\implies$ all $s_k \neq 0$. What is the loss?
- A training point's input value is changed slightly. What happens to the loss?
- The log of zero is not defined. Could this be a problem?

## Learning the parameters: $W, \mathbf{b}$

- Have training data $\mathcal{D}$.
- Have scoring function:

$$\mathbf{s} = f(\mathbf{x}; W, \mathbf{b}) = W\mathbf{x} + \mathbf{b}$$

- We have a choice of loss functions

$$l_{\text{softmax}}(\mathbf{x}, y, W, \mathbf{b}) = -\log\left(\frac{\exp(s_y)}{\sum_{k=1}^{C} \exp(s_k)}\right)$$

$$l_{\text{svm}}(\mathbf{x}, y, W, \mathbf{b}) = \sum_{\substack{j=1 \\ j \neq y}}^{C} \max(0, s_j - s_y + 1)$$

- Complete training loss

$$L(W, \mathbf{b}; \mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x}, y) \in \mathcal{D}} l_{\text{softmax(svm)}}(W, \mathbf{b}; \mathbf{x}, y) + \lambda R(W)$$

## Learning the parameters: $W, \mathbf{b}$

- Learning $W, \mathbf{b}$ corresponds to solving the optimization problem

$$W^*, \mathbf{b}^* = \arg\min_{W, \mathbf{b}} L(\mathcal{D}, W, \mathbf{b})$$

where

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- Know how to solve this! **Mini-batch gradient descent**.
- To implement mini-batch gradient descent need
  - to compute gradient of the loss $l_{\text{softmax(svm)}}(\mathbf{x}, y, W, \mathbf{b})$ and $R(W)$
  - Set the hyper-parameters of the mini-batch gradient descent procedure.

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## Next Lecture

We will cover how to compute these gradients using back-propagation.


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