Kyoto University

Statistical Learning Theory
- Classification -

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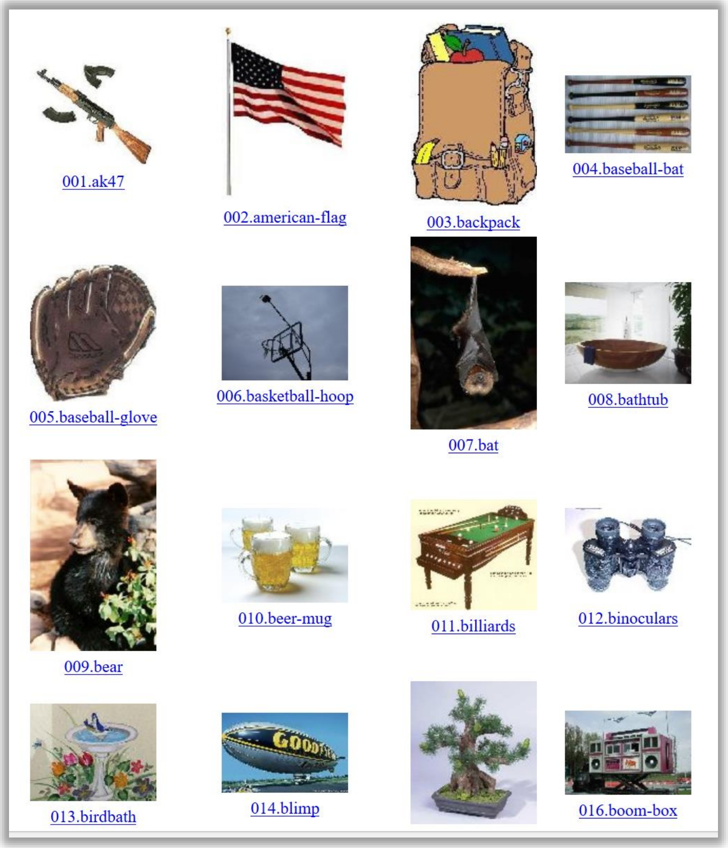
Classification

Classification: Supervised learning for predicting discrete variable

- Goal: Obtain a function $f: \mathcal{X} \to \mathcal{Y}$ ($\mathcal{Y}$: discrete domain)
  - E.g. $x \in \mathcal{X}$ is an image and $y \in \mathcal{Y}$ is the type of object appearing in the image
  - Two-class classification: $\mathcal{Y} = \{+1, -1\}$
- Training dataset: N pairs of an input and an output $\{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(N)}, y^{(N)})\}$



http://www.vision.caltech.edu/Image_Datasets/Caltech256/

Some applications of classification:
From binary to multi-class classification

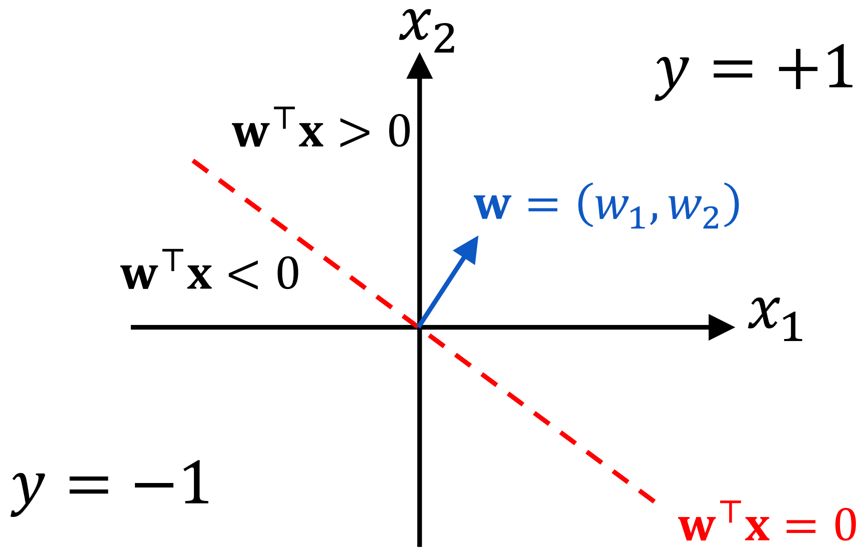
- Binary (two-class)classification:
  - Purchase prediction: Predict if a customer $\mathbf{x}$ will buy a particular product $(+1)$ or not (-1)
  - Credit risk prediction: Predict if a obligor $\mathbf{x}$ will pay back a debt $(+1)$ or not (-1)
- Multi-class classification ($\neq$ Multi-label classification):
  - Text classification: Categorize a document $\mathbf{x}$ into one of several categories, e.g., {politics, economy, sports, ...}
  - Image classification: Categorize the object in an image $\mathbf{x}$ into one of several object names, e.g., {AK5, American flag, backpack, ...}
  - Action recognition: Recognize the action type ({running, walking, sitting, ...}) that a person is taking from sensor data $\mathbf{x}$

Model for classification: Linear classifier

- Linear (binary) classification model:

$$y = \mathrm{sign}(\mathbf{w}^\top \mathbf{x}) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D)$$

  - $|\mathbf{w}^\top \mathbf{x}|$ indicates the intensity of belief
  - $\mathbf{w}^\top \mathbf{x} = 0$ gives a separating hyperplane
  - $\mathbf{w}$: normal vector perpendicular to the separating hyperplane



Learning framework: Loss minimization and statistical estimation

- Two learning frameworks

  1. Loss minimization: $L(\mathbf{w}) = \sum_{i=1}^{N} \ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right)$
     - Loss function ℓ: directly handles utility of predictions
     - Regularization term $R(\mathbf{w})$
  2. Statistical estimation (likelihood maximization): $L(\mathbf{w}) = \prod_{i=1}^{N} f_{\mathbf{w}}(y^{(i)} | \mathbf{x}^{(i)})$
     - Probabilistic model: generation process of class labels
     - Prior distribution $P(\mathbf{w})$

- They are often equivalent : { Loss = Probabilistic model; Regularization = Prior }

Classification problem in loss minimization framework: Minimize loss function + regularization term

- Minimization problem: $\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}} L(\mathbf{w}) + R(\mathbf{w})$
  - Loss function $L(\mathbf{w})$: Fitness to training data
  - Regularization term $R(\mathbf{w})$: Penalty on the model complexity to avoid overfitting to training data (usually norm of $\mathbf{w}$)
- Loss function should reflect the number of misclassifications on training data
  - Zero-one loss:

Correct classification

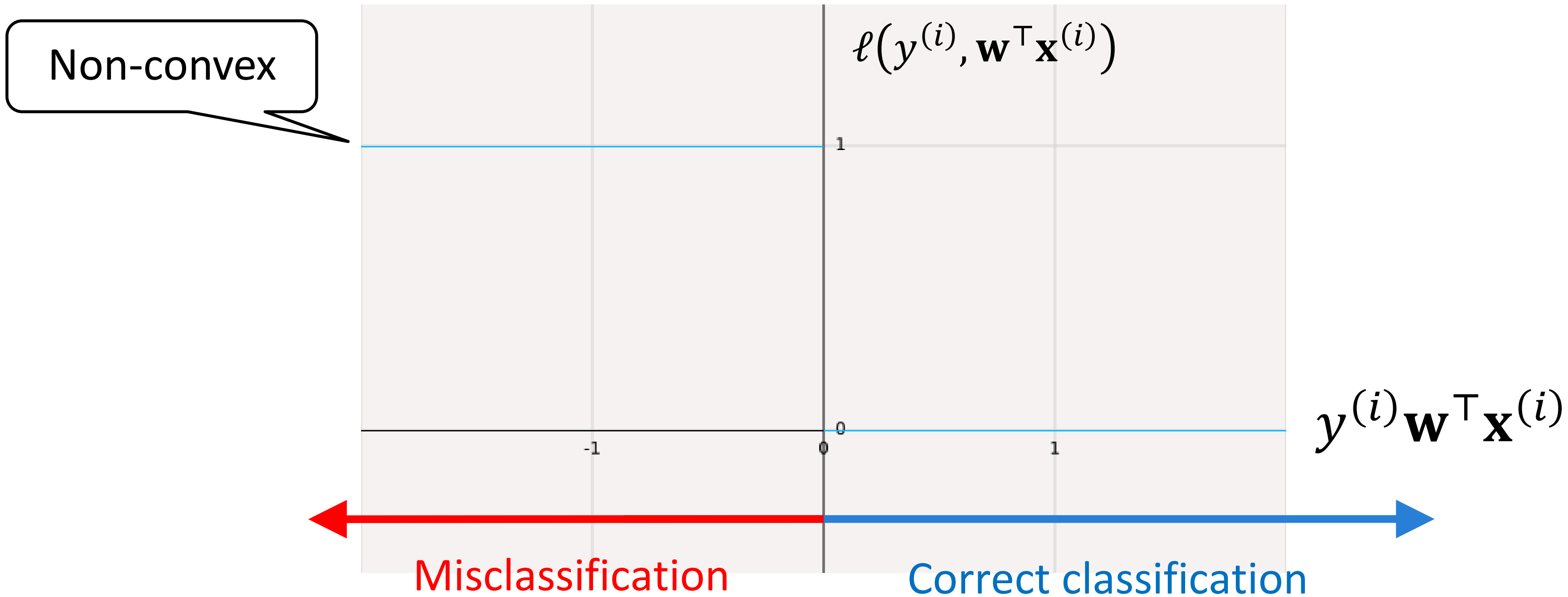
$$\ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right) = \begin{cases} 0 & \left(y^{(i)} = \mathrm{sign}\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) \\ 1 & \left(y^{(i)} \neq \mathrm{sign}\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) \end{cases}$$

Incorrect classification

Zero-one loss: Number of misclassification is hard to minimize

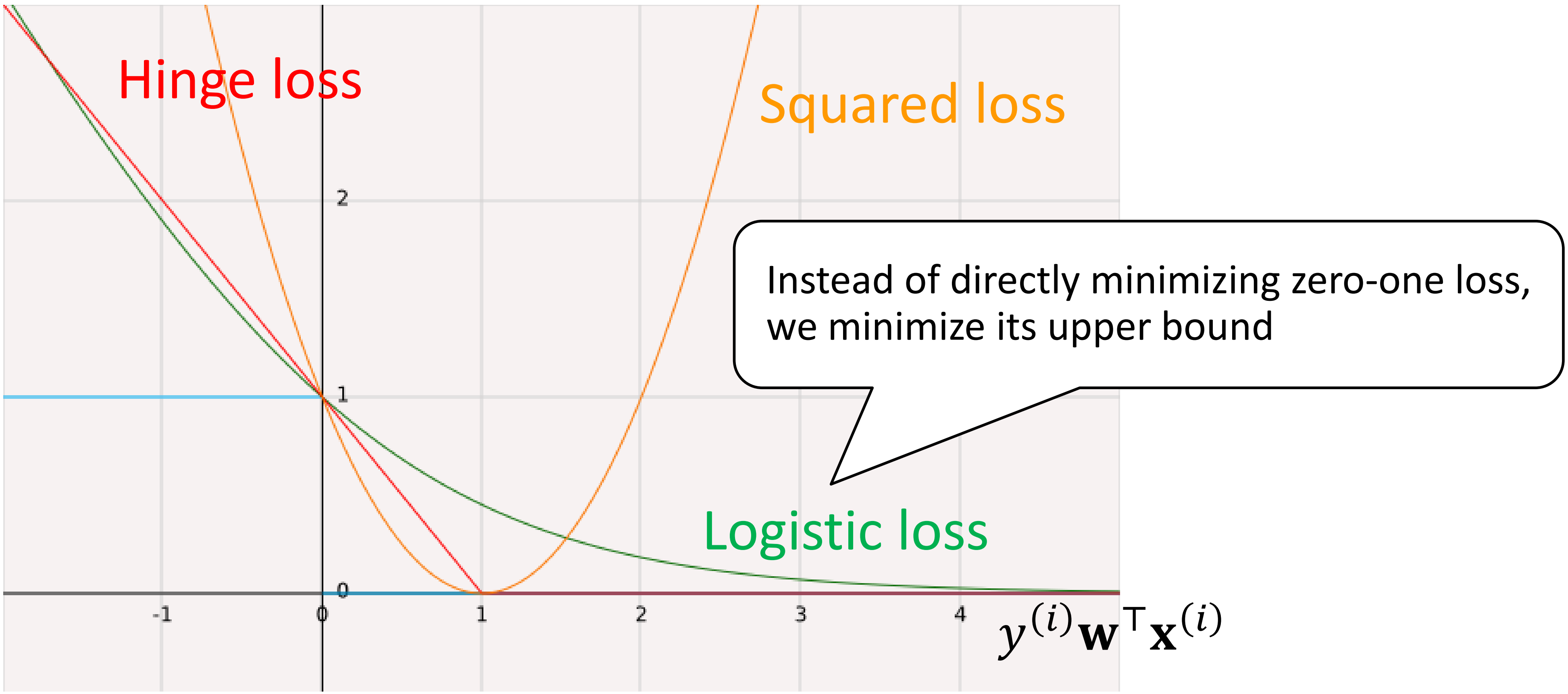
- Zero-one loss: $\ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right) = \begin{cases} 0 & \left(y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)} > 0\right) \\ 1 & \left(y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)} \leq 0\right) \end{cases}$

- Non-convex function is hard to optimize directly



Convex surrogates of zero-one loss: Different functions lead to different learning machines

- Convex surrogates: Upper bounds of zero-one loss
  - Hinge loss → SVM, Logistic loss → logistic regression, ...



Logistic regression

Logistic regression:
Minimization of logistic loss is a convex optimization

- Logistic loss:

$$\ell\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right) = \frac{1}{\ln 2} \ln\left(1 + \exp\left(-y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)}\right)\right)$$

- (Regularized) Logistic regression:

Convex

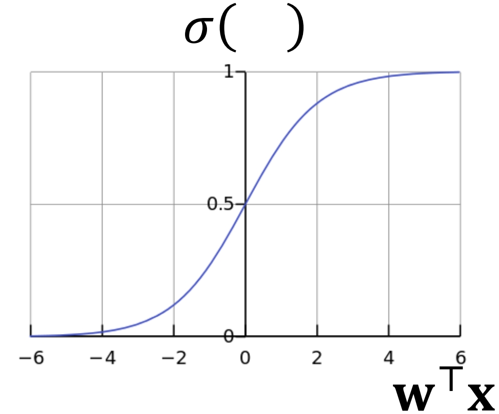
$$\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}} \sum_{i=1}^{N} \ln\left(1 + \exp\left(-y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) + \lambda \|\mathbf{w}\|_2^2$$

Statistical interpretation: Logistic loss min. as MLE of logistic regression model

- Minimization of logistic loss is equivalent to maximum likelihood estimation of logistic regression model

- Logistic regression model (conditional probability):

$$f_{\mathbf{w}}(y=1|\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{x})}$$



  - σ: Logistic function ($\sigma: \Re \to (0,1)$)

- Log likelihood:

$$L(\mathbf{w}) = \sum_{i=1}^{N} \log f_{\mathbf{w}}(y^{(i)}|\mathbf{x}^{(i)}) = -\sum_{i=1}^{N} \log\left(1+\exp\left(-y^{(i)}\mathbf{w}^\top \mathbf{x}\right)\right)$$

$$\left(= \sum_{i=1}^{N} \delta\left(y^{(i)}=1\right)\log\frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{x})} + \delta\left(y^{(i)}=-1\right)\log\left(1-\frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{x})}\right)\right)$$

Parameter estimation of logistic regression : Numerical nonlinear optimization

- Objective function of (regularized) logistic regression:

$$L(\mathbf{w}) = \sum_{i=1}^{N} \ln\left(1 + \exp\left(-y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) + \lambda \|\mathbf{w}\|_2^2$$

- Minimization of logistic loss / MLE of logistic regression model has no closed form solution

- Numerical nonlinear optimization methods are used
  - Iterate parameter updates: $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} + \mathbf{d}$

Parameter update : Find the best update minimizing the objective function

- By update $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} + \mathbf{d}$, the objective function will be:

$$L_{\mathbf{w}}(\mathbf{d}) = \sum_{i=1}^{N} \ln\left(1 + \exp\left(-y^{(i)}(\mathbf{w} + \mathbf{d})^{\top}\mathbf{x}^{(i)}\right)\right) + \lambda\|\mathbf{w} + \mathbf{d}\|_2^2$$

- Find $\mathbf{d}^*$ that minimizes $L_{\mathbf{w}}(\mathbf{d})$:

$$-\mathbf{d}^* = \mathrm{argmin}_{\mathbf{d}}\, L_{\mathbf{w}}(\mathbf{d})$$

Finding the best parameter update : Approximate the objective with Taylor expansion

- Taylor expansion:

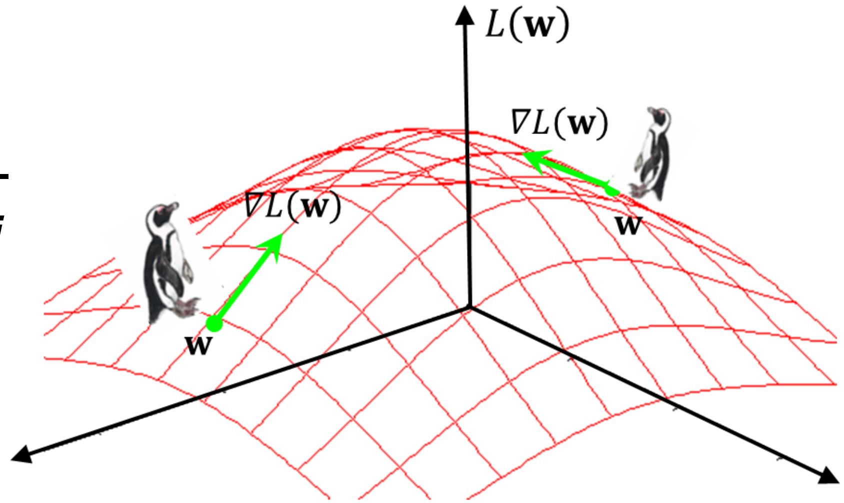
3rd-order term

$$L_{\mathbf{w}}(\mathbf{d}) = L(\mathbf{w}) + \mathbf{d}^{\top}\nabla L(\mathbf{w}) + \frac{1}{2}\mathbf{d}^{\top}\boldsymbol{H}(\mathbf{w})\mathbf{d} + O(\mathbf{d}^3)$$

– Gradient vector: $\nabla L(\mathbf{w}) = \left(\frac{\partial L(\mathbf{w})}{\partial w_1}, \frac{\partial L(\mathbf{w})}{\partial w_2}, \ldots, \frac{\partial L(\mathbf{w})}{\partial w_D}\right)^{\top}$

  - Steepest direction

– Hessian matrix: $[H(\mathbf{w})]_{i,j} = \frac{\partial^2 L(\mathbf{w})}{\partial w_i \partial w_j}$



Newton update : Minimizes the second order approximation

- Approximated Taylor expansion (neglecting the 3rd order term):

$$L_{\mathbf{w}}(\mathbf{d}) \approx L(\mathbf{w}) + \mathbf{d}^\top \nabla L(\mathbf{w}) + \frac{1}{2}\mathbf{d}^\top \boldsymbol{H}(\mathbf{w})\mathbf{d} \cancel{+ O(\mathbf{d}^3)}$$

- Derivative w.r.t. $\mathbf{d}$: $\frac{\partial L_{\mathbf{w}}(\mathbf{d})}{\partial \mathbf{d}} \approx \nabla L(\mathbf{w}) + \boldsymbol{H}(\mathbf{w})\mathbf{d}$

- Setting it to be $\mathbf{0}$, we obtain $\mathbf{d} = -\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$

- Newton update formula:

$$\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$$

Modified Newton update: Second order approximation + linear search

- The correctness of the update $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$ depends on the second-order approximation:

$$L_{\mathbf{w}}(\mathbf{d}) \approx L(\mathbf{w}) + \mathbf{d}^{\top}\nabla L(\mathbf{w}) + \frac{1}{2}\mathbf{d}^{\top}\boldsymbol{H}(\mathbf{w})\mathbf{d}$$

  – This is not actually true for most cases

- Use only the direction of $\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$ and update with $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$

- Learning rate $\eta > 0$ is determined by linear search:

$$\eta^{*} = \mathrm{argmax}_{\eta}\, L\big(\mathbf{w} - \eta\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})\big)$$

(Steepest) gradient descent: Simple update without computing inverse Hessian

- Computing the inverse of Hessian matrix is costly
  - Newton update: $\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \boldsymbol{H}(\mathbf{w})^{-1} \nabla L(\mathbf{w})$
- (Steepest) gradient descent:
  - Replacing $\boldsymbol{H}(\mathbf{w})^{-1}$ with $\boldsymbol{I}$ gives

$$\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \nabla L(\mathbf{w})$$

Gradient of objective function

  - $\nabla L(\mathbf{w})$ is the steepest direction
  - Learning rate η is determined by line search

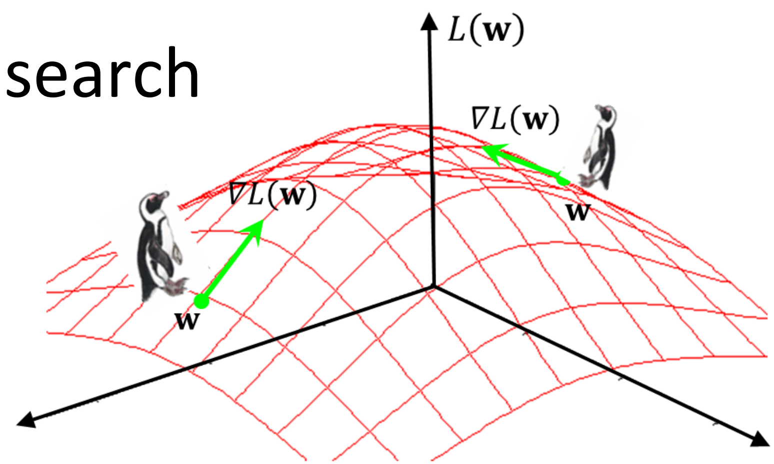
Summary:
Gradient descent

- Steepest gradient descent is the simplest optimization method:
- Update the parameter in the steepest direction of the objective function

$$\mathbf{w}^{\mathrm{NEW}} \leftarrow \mathbf{w} - \eta \nabla L(\mathbf{w})$$

– Gradient: $\nabla L(\mathbf{w}) = \left(\frac{\partial L(\mathbf{w})}{\partial w_1}, \frac{\partial L(\mathbf{w})}{\partial w_2}, \ldots, \frac{\partial L(\mathbf{w})}{\partial w_D} \right)^\top$

– Learning rate η is determined by line search



Example of gradient descent: Gradient of logistic regression

- $L(\mathbf{w}) = \sum_{i=1}^{N} \ln\left(1 + \exp\left(-y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}\right)\right)$

- $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \sum_{i=1}^{N} \frac{1}{1+\exp\left(-y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}\right)} \frac{\partial\left(1+\exp\left(-y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}\right)\right)}{\partial \mathbf{w}}$

$$= -\sum_{i=1}^{N} \frac{1}{1+\exp\left(-y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}\right)} \exp\left(-y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}\right) y^{(i)}\mathbf{x}^{(i)}$$

$$= -\sum_{i=1}^{N} \left(1 - f_{\mathbf{w}}\left(y^{(i)}|\mathbf{x}^{(i)}\right)\right) y^{(i)}\mathbf{x}^{(i)}$$

Can be easily computed with the current prediction probabilities

Mini batch optimization:
Efficient training using data subsets

- Objective function for N instances:
  $L(\mathbf{w}) = \sum_{i=1}^{N} \ell\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right) + \lambda R(\mathbf{w})$

- Its derivative $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \sum_{i=1}^{N} \frac{\partial \ell\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)}{\partial \mathbf{w}} + \lambda \frac{\partial R(\mathbf{w})}{\partial \mathbf{w}}$ needs $O(N)$ computation

- Approximate this with only one instance:
  $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} \approx N \frac{\partial \ell\left(\mathbf{w}^\top \mathbf{x}^{(j)}\right)}{\partial \mathbf{w}} + \lambda \frac{\partial R(\mathbf{w})}{\partial \mathbf{w}}$ (Stochastic approximation)

- Also we can do this with $1 < M < N$ instances:
  $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} \approx \frac{N}{M} \sum_{j \in \mathrm{MiniBatch}} \frac{\partial \ell\left(\mathbf{w}^\top \mathbf{x}^{(j)}\right)}{\partial \mathbf{w}} + \lambda \frac{\partial R(\mathbf{w})}{\partial \mathbf{w}}$ (Mini batch)

Model Evaluation

Model evaluation:
How can we know the “real” performance of a model?

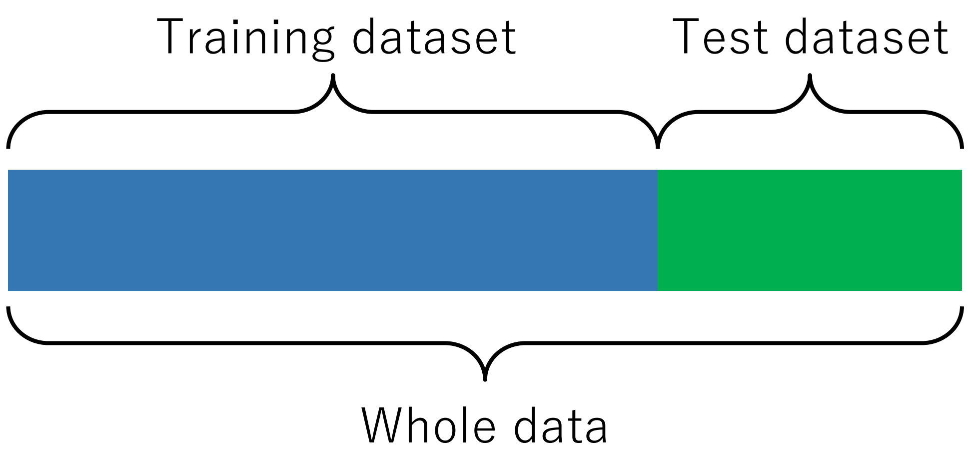
- Once you obtain a trained model, you want to deploy the model in your application
- How well will the model perform? - We are interested in the future performance of the obtained model when it is deployed
  - How many mistakes will the model make in future?
- Even the model performs perfectly on the training data, the same performance is not guaranteed for future data
- “Model evaluation” problem

The first principle:
Evaluation must use a dataset not used in training

- You *must not* evaluate your classifier based on the performance on the dataset you already used for training
- The performance of a model for the training data is not an estimate of its true performance
  - If you memorize all the answers of the training dataset, you will always be correct for them
  - … but there is no guarantee that you will be so for future data

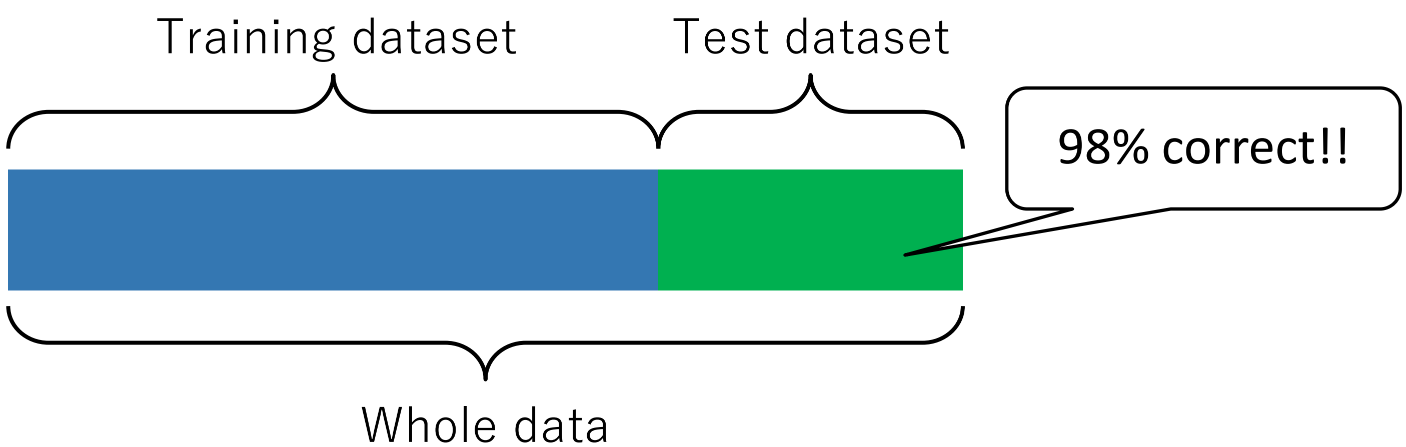
A simplest solution for model evaluation: Secure some data for performance evaluation

- Divide the dataset into a *training dataset* and a *test dataset*
  1. Train a classifier using the training dataset
  2. Evaluate its performance on the test dataset
- This is simulating a real application scenario using only the dataset at hand (without using real future data)



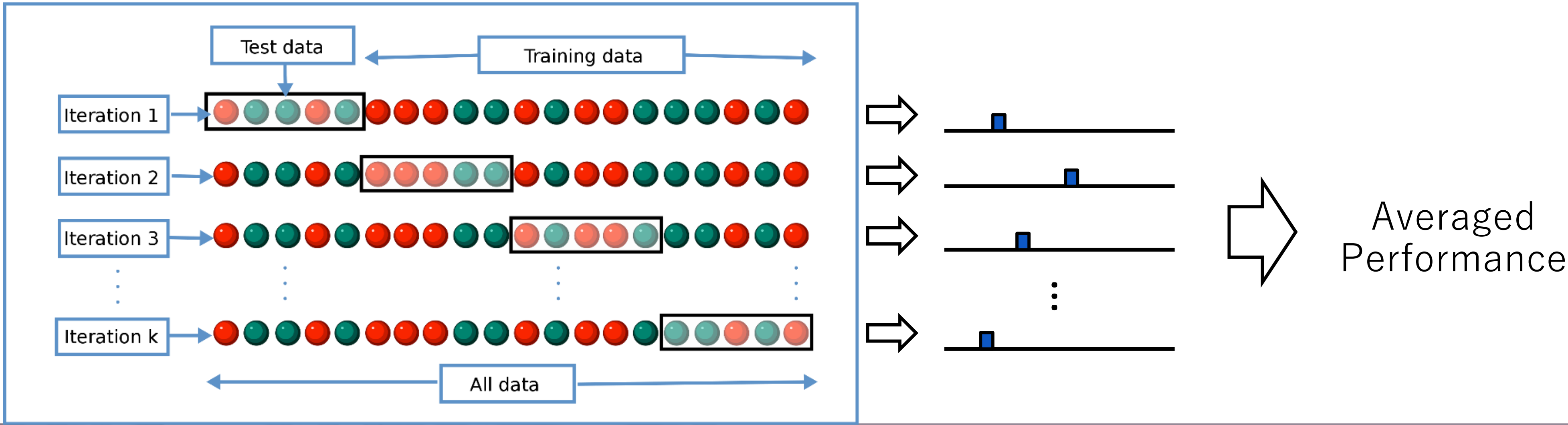
Reliability of test performance: How much can we trust the estimated performance?

- Now you have 98% prediction accuracy on your test data
  … How much can you believe this?
  - Isn't it simply a lucky coincidence?
- Why not just repeat the random separation of training data and test data?



A statistical framework for performance evaluation: Cross validation

- Divide a given dataset into K non-overlapping sets
  - Use $K-1$ of them for training
  - Use the remaining one for testing
- Changing the test dataset results in K measurements
  - Take their average to get a final performance estimate



 https://en.wikipedia.org/wiki/Cross-validation_(statistics)

Model Selection

Model selection:
How can we tune the hyperparameters?

- We often have some hyper-parameters to be tuned so that the final performance gets better
  - E.g. Training target of the ridge regression:

Hyperparameter

$$\mathrm{minimize}_{\mathbf{w}} \ \|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$$

  - Hyper-parameters are not optimized in the training
    - Joint optimization just gives a trivial solution $\lambda = 0$

Statistical framework for tuning hyper-parameters: Cross validation (again)

- (K-fold) cross validation can also be used for determining hyper parameters
  - Use $K - 1$ of K sets for training models for various hyper-parameter settings
  - Use the remaining one for testing
  - Choose the hyper-parameter setting with the best averaged performance
    - Note that this is **NOT** the estimate of its final performance

Double-loop cross validation: Tuning hyper-parameters and performance evaluation at the same time

- Sometimes you want to do *both* hyper-parameter tuning and estimation of future performance
- Doing both with one K-fold cross validation is guilty 
  - You saw the test dataset for tuning hyper-parameters
- Double-loop cross validation:
  - Outer loop for performance evaluation
  - Inner loop for hyper-parameter tuning
  - High computational costs…

A simple alternative of double-loop cross validation: "Development set" approach

- A simple alternative for the double-loop cross validation
- "Development set" approach
  - Use $K - 2$ of K sets for training
  - Use one for tuning hyper-parameters
  - Use one for testing