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KYOTO UNIVERSITY

Statistical Learning Theory
- Classification -

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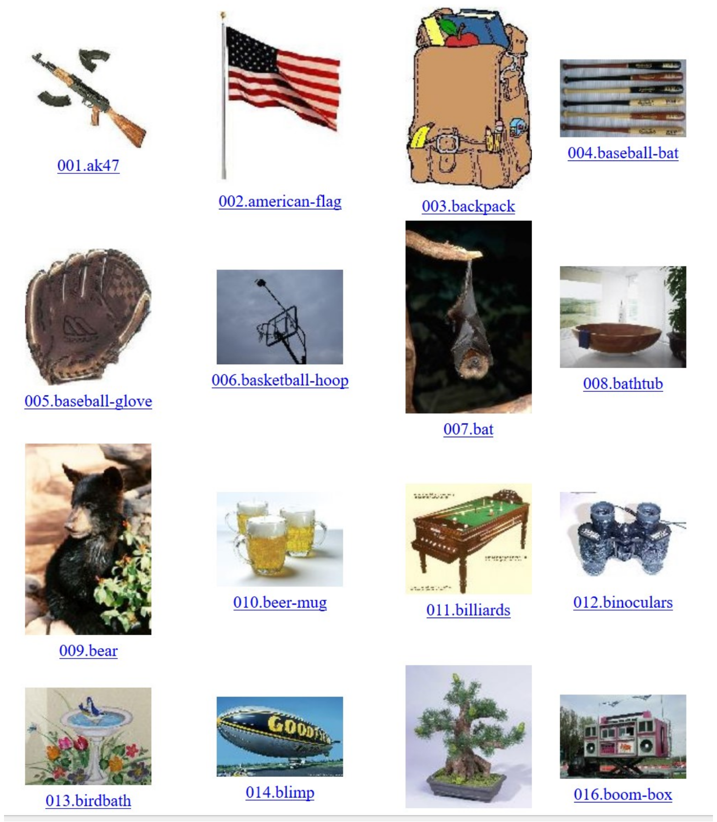
Classification

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

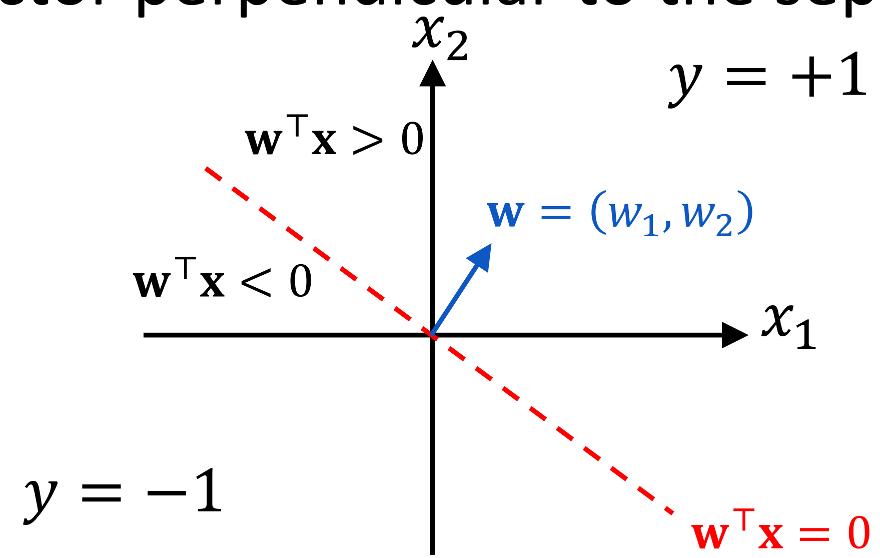
- Binary (two-class)classification:
  - Purchase prediction: Predict if a customer $\mathbf{x}$ will buy a particular product (+1) or not (-1)
  - Credit risk prediction: Predict if a obligor $\mathbf{x}$ will pay back a debt (+1) or not (-1)
- Multi-class classification:
  - Text classification: Categorize 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 classification: Liner regression 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 hyperplace



Learning framework: Loss minimization and statistical estimation

- Two learning frameworks

  1. Loss minimization: $L(\mathbf{w}) = \sum_{i=1}^{N} \ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)};\ \mathbf{w}\right)$
     - Loss function $\ell^{(i)}$: directly handles utility of predictions
     - Regularization term $R(\mathbf{w})$
  2. Statistical estimation (likelihood maximization):
     $L(\mathbf{w}) = \prod_{i=1}^{N} f(y^{(i)} | \mathbf{x}^{(i)}, \mathbf{w})$
     - Probabilistic model: Noise assumptions are clear
     - 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:

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

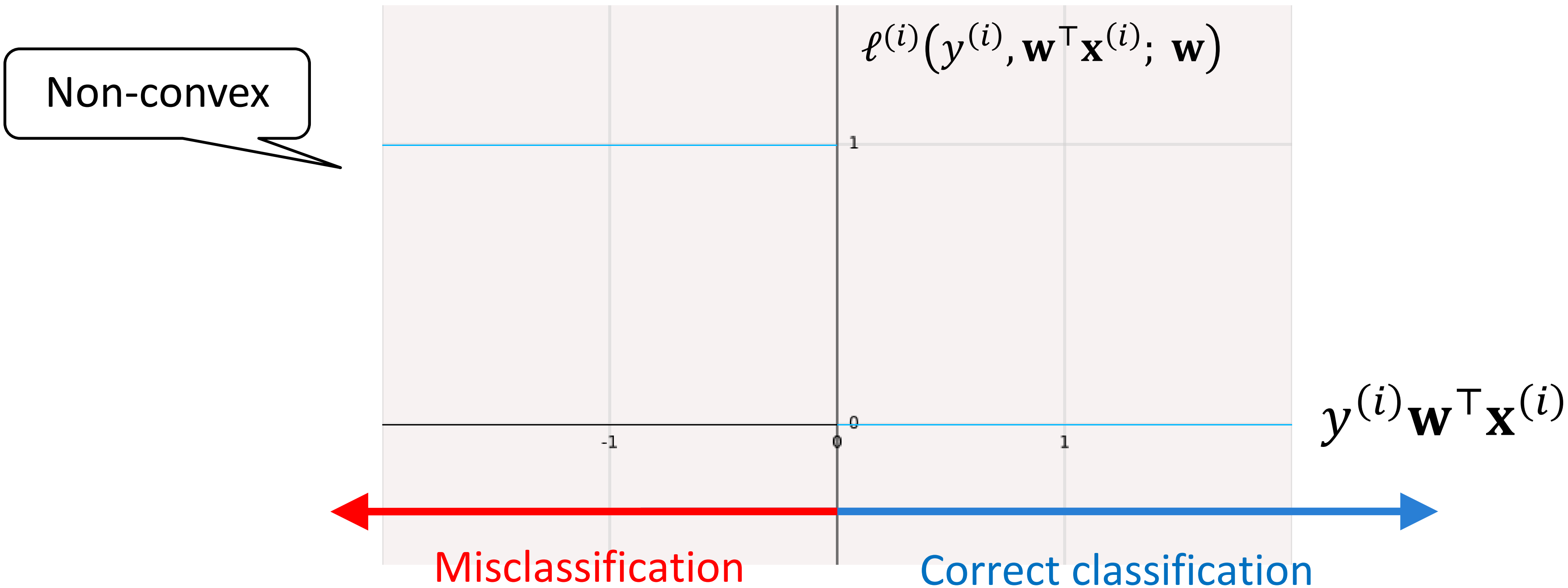
Correct classification

Incorrect classification

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

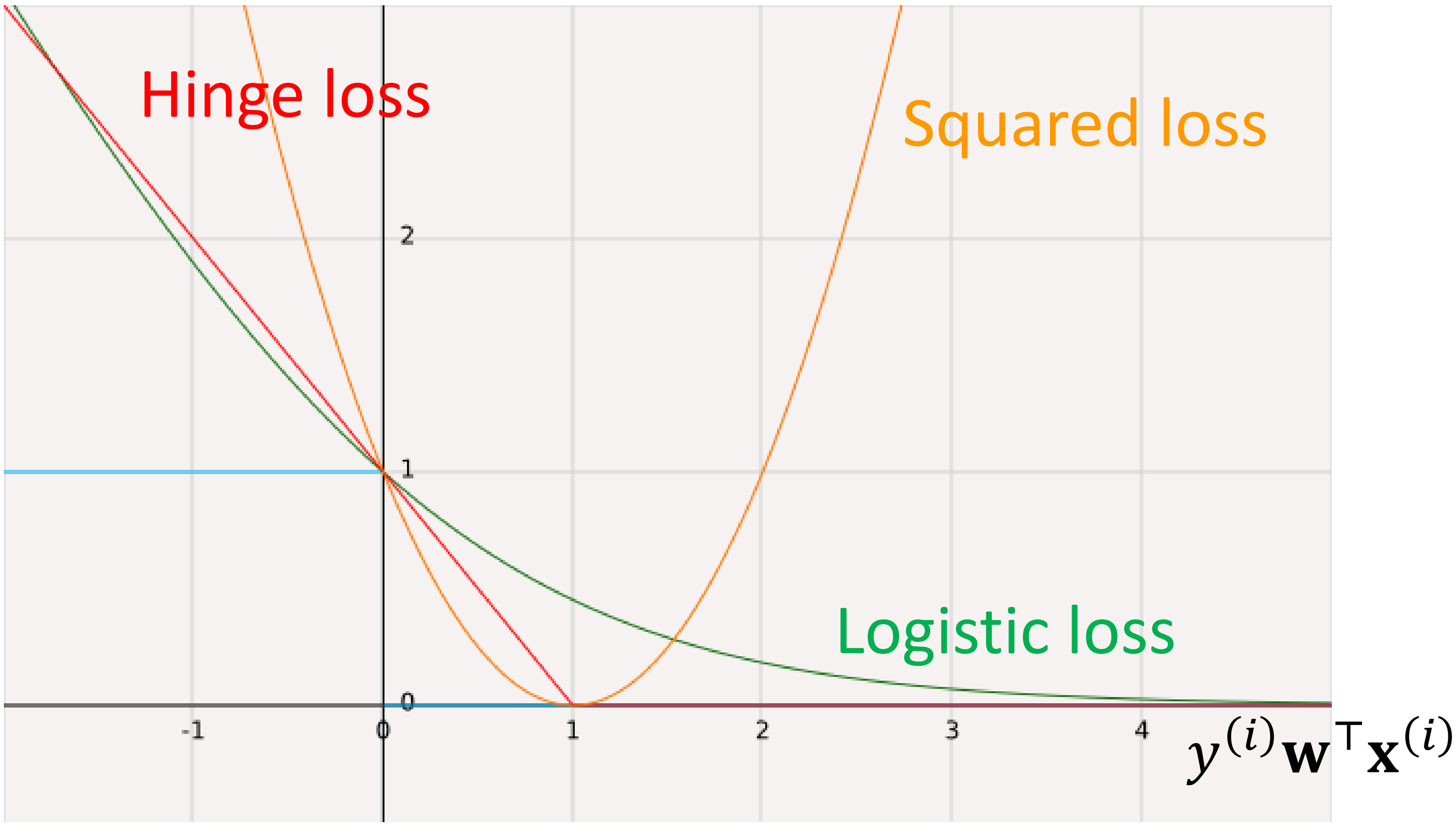
- Zero-one loss: $\ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)};\ \mathbf{w}\right) = \begin{cases} 0 & \left(y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} > 0\right) \\ 1 & \left(y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} \leq 0\right) \end{cases}$

- 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

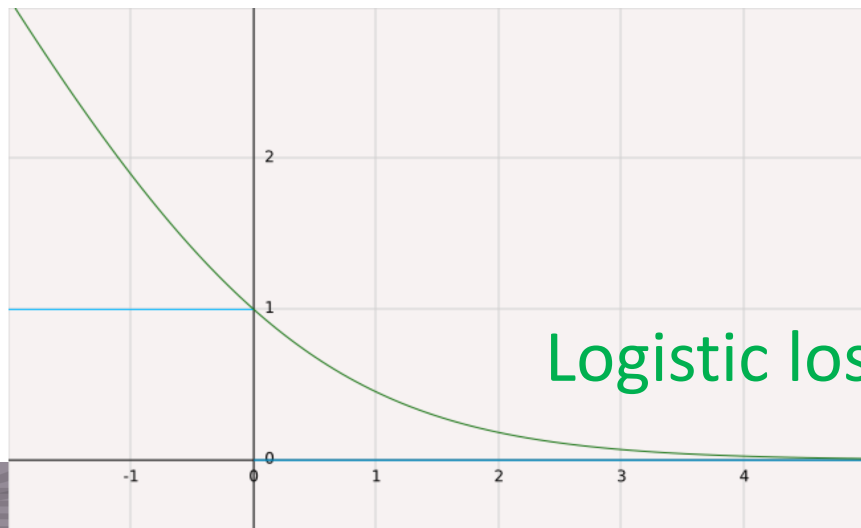
- Logistic loss:

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

- (Regularized) Logistic regression:

Convex

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

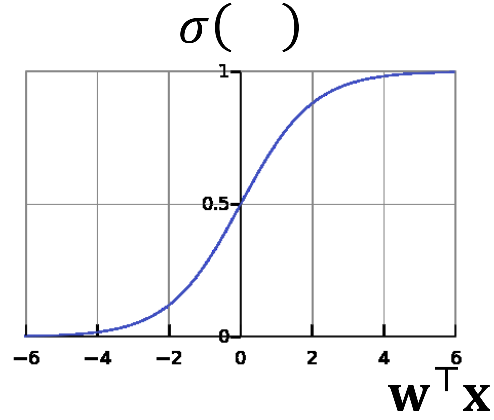


Statistical interpretation: Logistic loss min. as MLE of logistic regression model

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

- Logistic regression model (conditional probability):

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



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

- Log likelihood:

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

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

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:

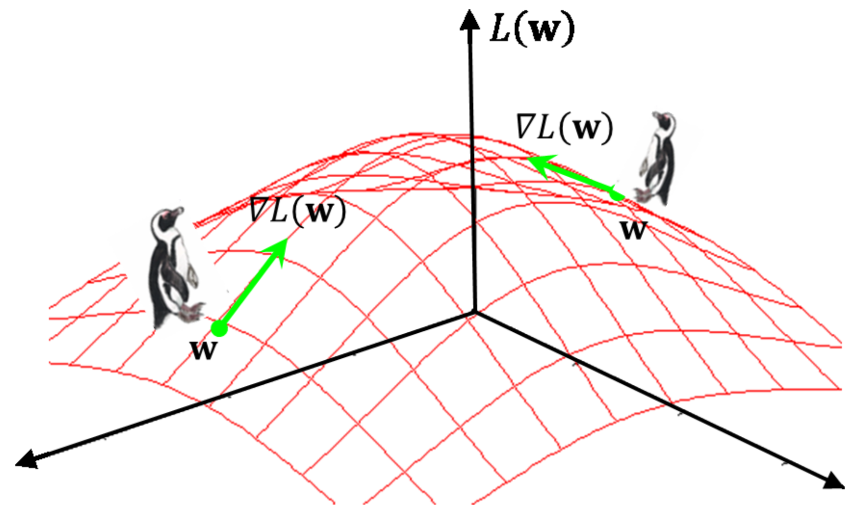
3rd-order term

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

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

  - Steepest direction

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



Newton update :
Minimizes the second order approximation

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

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

- 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 $\mathbf{0}$, $\mathbf{d} = -\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$

- 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:

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

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 $\boldsymbol{I}$ will give

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

Gradient of objective function

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

(Supplement) :
Computing the gradient of logistic regression

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

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

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

$$= -\sum_{i=1}^{N} (1 - f(y^{(i)}|\mathbf{x}^{(i)}, \mathbf{w}))\, y^{(i)}\mathbf{x}^{(i)}$$

Can be easily computed with the current prediction probabilities

Mini batch:
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)

Support Vector Machine and Kernel Methods

Support vector machine: One of the most successful learning methods

- One of the most important achievements in machine learning
  - Proposed in 1990s by Cortes & Vapnik
  - Suitable for small to middle sized data
- A learning algorithm of linear classifiers
  - Based on "margin maximization" principle
  - Understood as hinge loss + L2-regularization
- Kernel methods: Capable of non-linear classification through kernel functions
  - SVM is one of the kernel methods

Loss function of support vector machine: Hinge loss

- In SVM, we use hinge loss as a convex upper bound of 0-1 loss

$$\ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)};\ \mathbf{w}\right) = \max\{1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}, 0\}$$

- Squared hinge loss $\max\{\left(1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}\right)^2, 0\}$ is also sometimes used

Two formulations of SVM training:
Soft-margin SVM and hard margin SVM

- When we use L2 regularization, we have "soft-margin" SVM:

$$\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}} \sum_{i=1}^{N} \max\{1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}, 0\} + \lambda \|\mathbf{w}\|_2^2$$

  – This is a convex optimization problem ☺

- With constraint on the loss, we have "hard-margin" SVM:

$$\mathbf{w}^* = \mathrm{argmin}_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|_2^2 \text{ s.t. } \sum_{i=1}^{N} \max\{1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)}, 0\} = 0$$

  – Equivalently, the constraint is written as
    $1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)} \leq 0$ (for all $i = 1,2, \dots, N$)

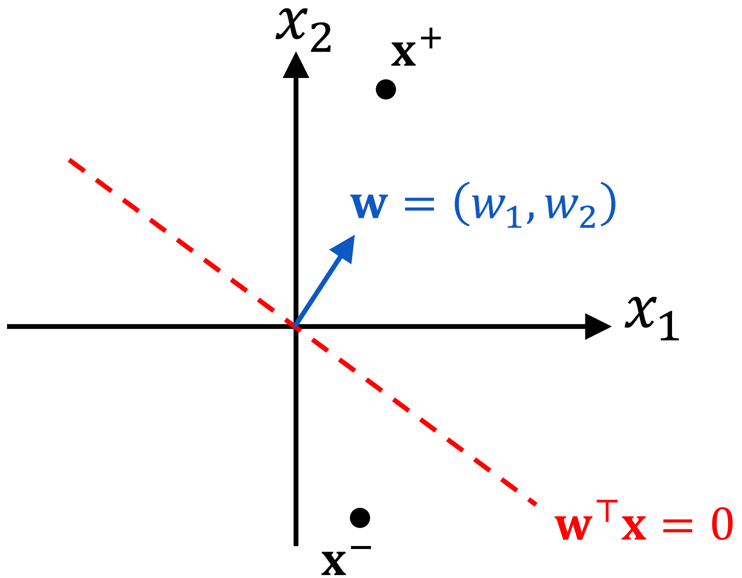
  – The originally proposed SVM formulation was in this form

Geometric interpretation: Hard-margin SVM maximizes the margin

- $\min \frac{1}{2} \| \mathbf{w} \|_2^2 \leftrightarrow \max \frac{1}{\|\mathbf{w}\|_2}$ ($\frac{1}{\|\mathbf{w}\|_2}$ is called *margin*)
- $\frac{\mathbf{w}^\top(\mathbf{x}^+ - \mathbf{x}^-)}{\|\mathbf{w}\|_2}$: Sum of distances between separating hyperplane and a positive instance $\mathbf{x}^+$ and a negative instance $\mathbf{x}^-$
- Since $1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)} \leq 0 \;\; \forall i$,

$\frac{\mathbf{w}^\top(\mathbf{x}^+ - \mathbf{x}^-)}{\|\mathbf{w}\|_2}$ is lower bounded $\frac{2}{\|\mathbf{w}\|_2}$

They can be taken as the closest instance to the separating hyperplane



Solution of hard-margin SVM (Step I): Introducing Lagrange multipliers

- $\min_{\mathbf{w}} \frac{1}{2} \| \mathbf{w} \|_2^2$ s.t. $1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} \leq 0 \ (i = 1,2, \dots, N)$

- Lagrange multipliers $\{\alpha_i\}_i$:

$$\min_{\mathbf{w}} \max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\dots,\alpha_N)\geq 0} \left(\frac{1}{2} \| \mathbf{w} \|_2^2 + \sum_{i=1}^{N} \alpha_i \left(1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}\right) \right)$$

  – If $1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} > 0$ for some i, we have $\alpha_i = \infty$
    - The objective function becomes ∞, that cannot be optimal
  – If $1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} \leq 0$ for some i, we have either $\alpha_i = 0$ or $\left(1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}\right) = 0$, i.e. objective function remains the same as the original one ($\frac{1}{2} \| \mathbf{w} \|_2^2$)

Solution of hard-margin SVM (Step II): Dual formulation as a quadratic programming problem

- By changing the order of min and max:

$$\min_{\mathbf{w}} \max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\geq 0} \left(\frac{\| \mathbf{w} \|_2^2}{2} + \sum_{i=1}^{N} \alpha_i \left(1 - y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)}\right) \right)$$

$$\Downarrow$$

$$\max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\geq 0} \min_{\mathbf{w}} \left(\frac{\| \mathbf{w} \|_2^2}{2} + \sum_{i=1}^{N} \alpha_i \left(1 - y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)}\right) \right)$$

- Solving min gives $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^{(i)} \mathbf{x}^{(i)}$, which finally results in

$$\max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\geq 0} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} {\mathbf{x}^{(i)}}^\top \mathbf{x}^{(j)}$$

Support vectors:
SVM model depends only on support vectors

- The dual problem:

$$\max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\geq 0} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} {\mathbf{x}^{(i)}}^\top \mathbf{x}^{(j)}$$

$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^{(i)} \mathbf{x}^{(i)}$

- Support vectors: the set of i such that $\alpha_i > 0$
  - For such i, $1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)} = 0$ holds
  - They are the closest instance to the separating hyperplane
- Non-support vectors ($\alpha_i = 0$) do not appear in the model:
  $\mathbf{w}^\top \mathbf{x} = \sum_{j=1}^{N} \alpha_j y^{(j)} {\mathbf{x}^{(j)}}^\top \mathbf{x}$

Solution of soft-margin SVM: Additional constraints

- Equivalent formulation of soft-margin SVM:

$$\min_{\mathbf{w}} \|\mathbf{w}\|_2^2 + C\sum_{i=1}^{N} e_i$$

Hinge loss (Slack variable)

$$\text{s.t. } 1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)} \le e_i$$

$$(i = 1, 2, \dots, N)$$

- Similar dual problem with additional constraints:

$$\max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\dots,\alpha_N)\ge 0} \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y^{(i)}y^{(j)}\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$$

$$0 \le \alpha_i \le C \quad (i = 1, 2, \dots, N)$$

Kernel methods: Data access through kernel function

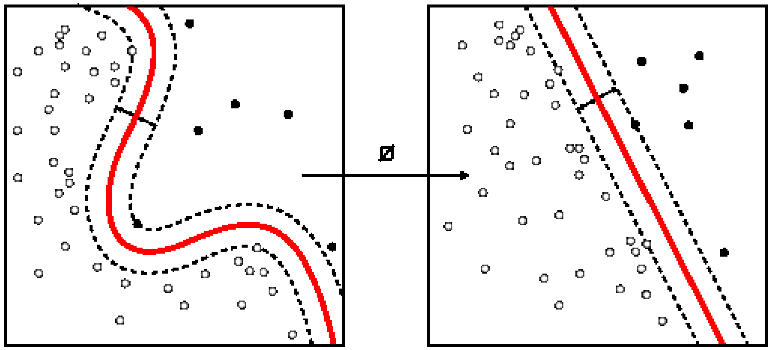
- The dual form objective function and the classifier access to data always through inner products $\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$
  - The inner product $\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$ is considered as similarity
- Can we use some similarity function $K\left(\mathbf{x}^{(i)},\mathbf{x}^{(j)}\right)$ instead of $\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$? – Yes (under certain conditions)

$$\max_{\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\geq 0} \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i}^{N}\sum_{j}^{N}\alpha_i\alpha_j y^{(i)}y^{(j)}K\left(\mathbf{x}^{(i)},\mathbf{x}^{(j)}\right)$$

  - Model : $\mathbf{w}^\top\mathbf{x} = \sum_{j=1}^{N}\alpha_j y^{(j)}K\left(\mathbf{x}^{(j)},\mathbf{x}\right)$

Kernel functions:
Introducing non-linearity in linear models

- Consider a (nonlinear) mapping $\boldsymbol{\phi}: \Re^{D} \rightarrow \Re^{D'}$
  - D-dimensional space to $D'(\gg D)$-dimensional space
  - Vector $\mathbf{x}$ is mapped to a high-dimensional vector $\boldsymbol{\phi}(\mathbf{x})$
- Define kernel $K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right)^{\top} \boldsymbol{\phi}(\mathbf{x}^{(j)})$
- SVM is a linear classifier in the D'-dimensional space, while is a non-linear classifier in the original space



https://en.wikipedia.org/wiki/Support_vector_machine#/media/File:Kernel_Machine.svg

Advantage of kernel methods: Computational efficiency in terms of input dimensions

- Advantage of using kernel function

$$K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right)^{\top} \boldsymbol{\phi}(\mathbf{x}^{(j)})$$

- Even if $\boldsymbol{\phi}$ is high-dimensional (possibly infinite dimensional), as far as its inner product $\boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right)^{\top} \boldsymbol{\phi}(\mathbf{x}^{(j)})$ is given as an efficiently computable function, the dimension of $\boldsymbol{\phi}$ does not matter

- Problem size:

$$D(\text{number of dimensions}) \rightarrow N(\text{number of data})$$

  – Advantageous when $\boldsymbol{\phi}$ is especially high or infinite dimensional

Example of kernel functions: Polynomial kernel can consider high-order cross terms

- Combinatorial features: Not only the original features $x_1, x_2, \ldots, x_D$, use their combinations (i.e. products)
  - Exponential number of dimensions wrt d

- Polynomial kernel: $K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \left(\mathbf{x}^{(i)\top}\mathbf{x}^{(j)} + c\right)^d$
  - E.g. $c = 0, d = 2$, two dimensional case

$$\mathbf{x}^{(i)} = \begin{pmatrix} x_1^{(i)} \\ x_2^{(i)} \end{pmatrix}$$

$$K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \left(x_1^{(i)} x_1^{(j)} + x_2^{(i)} x_2^{(j)}\right)^2$$

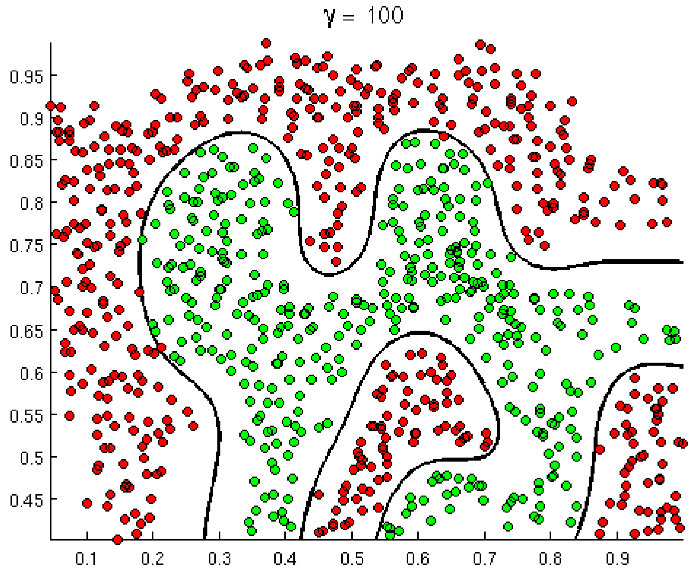
$$= \left(x_1^{(i)2}, x_2^{(i)2}, \sqrt{2} x_1^{(i)} x_2^{(i)}\right)\left(x_1^{(j)2}, x_2^{(j)2}, \sqrt{2} x_1^{(j)} x_2^{(j)}\right)$$

  - Note that it can be computed in $O(D)$

Example of kernel functions:
Gaussian kernel with infinite feature space

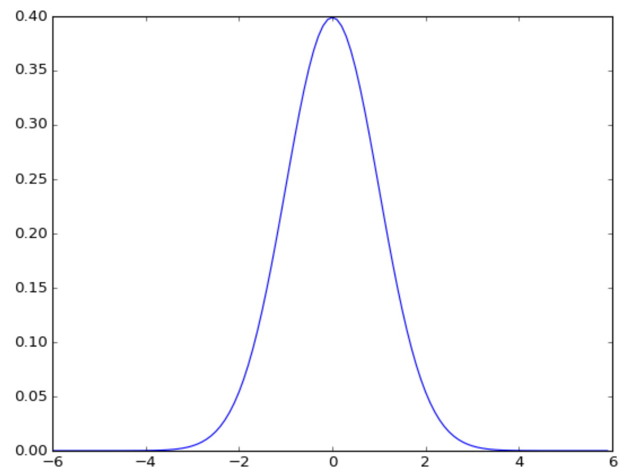
- Gaussian kernel (RBF kernel): $K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma}\right)$
  - Can be interpreted as an inner product in an infinite-dimensional space

Discrimination surface with Gaussian kernel



http://openclassroom.stanford.edu/MainFolder/DocumentPage.php?course=MachineLearning&doc=exercises/ex8/ex8.html

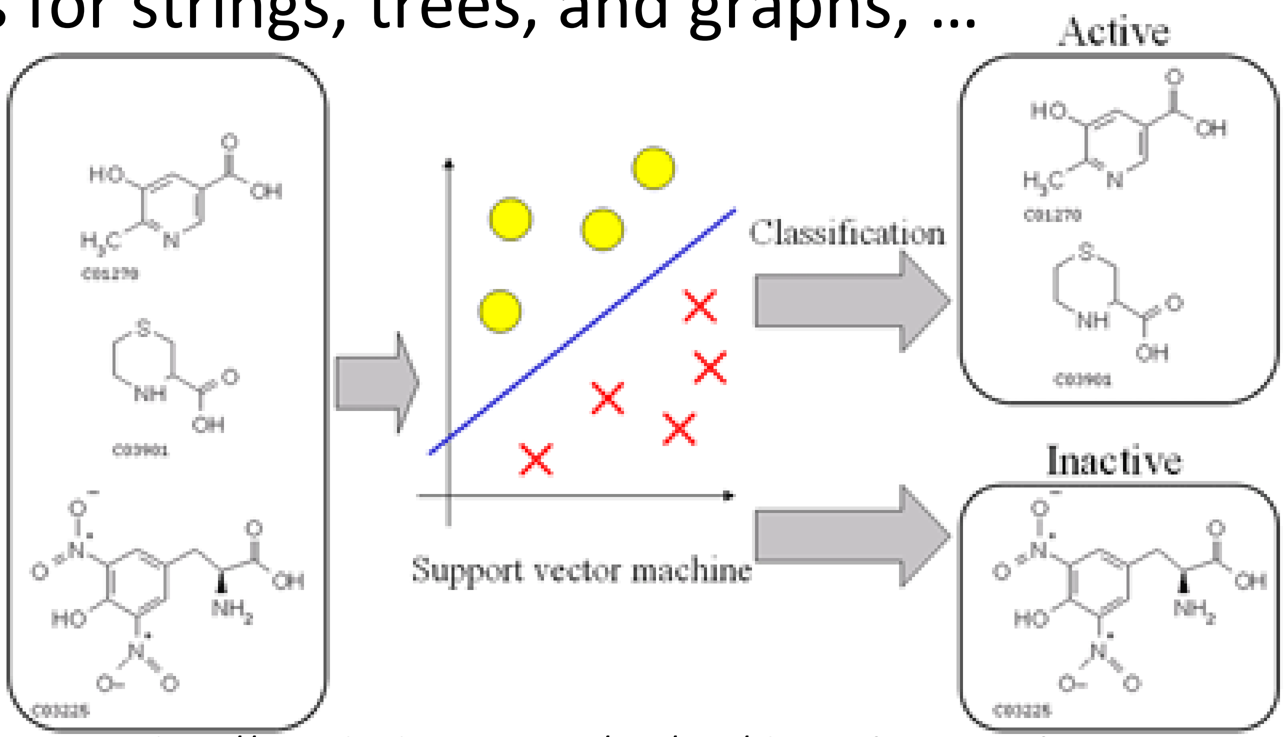
Gaussian kernel (RBF kernel)



$\| \mathbf{x}_i - \mathbf{x}_j \|_2^2$

Kernel methods for non-vectorial data:
Kernels for sequences, trees, and graphs

- Kernel methods can handle any kinds of objects (even non-vectorial objects) as long as efficiently computable kernel function is available
  - Kernels for strings, trees, and graphs, …



http://www.bic.kyoto-u.ac.jp/coe/img/akutsu_fig_e_02.gif

Representer theorem:
Theoretical underpinning of kernel methods

- Can we use some similarity function as a kernel function?
  - Yes (under certain conditions)

- Kernel methods rely on the fact that the optimal parameter is represented as a linear combination of input vectors:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^{(i)} \mathbf{x}^{(i)}$$

  - Gives the dual form $\mathbf{w}^\top \mathbf{x} = \sum_{j=1}^{N} \alpha_j y^{(j)} \mathbf{x}^{(j)\top} \mathbf{x}$

- Representer theorem:
  This is guaranteed under L2-regularization

(Simple) proof of representer theorem: Obj. func. depends only on the linear combination

- Assumption: Loss $\ell^{(i)}$ for i-th data depends only on $\mathbf{w}^\top \mathbf{x}^{(i)}$
  - Objective function: $L(\mathbf{w}) = \sum_{i=1}^{N} \ell^{(i)}\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right) + \lambda \|\mathbf{w}\|_2^2$
- Divide the optimal parameter $\mathbf{w}^*$ into two parts $\mathbf{w} + \mathbf{w}^\perp$:
  - $\mathbf{w}$: Linear combination of input data $\left\{\mathbf{x}^{(i)}\right\}_i$
  - $\mathbf{w}^\perp$: Other parts (orthogonal to all input data)
- $L(\mathbf{w}^*)$ depends only on $\mathbf{w}$: $\sum_{i=1}^{N} \ell^{(i)}\left({\mathbf{w}^*}^\top \mathbf{x}^{(i)}\right) + \lambda \|\mathbf{w}^*\|_2^2$

$$= \sum_{i=1}^{N} \ell^{(i)}\left(\mathbf{w}^\top \mathbf{x}^{(i)} + \underbrace{{\mathbf{w}^\perp}^\top \mathbf{x}^{(i)}}_{=0}\right) + \lambda\left(\|\mathbf{w}\|_2^2 + \underbrace{2\mathbf{w}^\top \mathbf{w}^\perp}_{=0} + \underbrace{\|\mathbf{w}^\perp\|_2^2}_{\text{Minimized to } = 0}\right)$$

Primal objective function:

Kernel representation is also available in the primal form

- Primal objective function of SVM:

$$L(\mathbf{w}) = \sum_{i=1}^{N} \max\{1 - y^{(i)}\mathbf{w}^\top \mathbf{x}^{(i)}, 0\} + \lambda \|\mathbf{w}\|_2^2$$

- Primal objective function using kernel:

Using
$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^{(i)} \mathbf{x}^{(i)}$

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \max\{1 - y^{(i)} \sum_{j=1}^{N} \alpha_j y^{(j)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right), 0\} + \lambda \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)$$

Support vector regression:
Use ϵ-insensitive loss instead of hinge loss

- Instead of the hinge loss, use ϵ-insensitive loss:

$$\ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)};\ \mathbf{w}\right) = \max\{\left|y_i - \mathbf{w}^\top \mathbf{x}^{(i)}\right| - \epsilon, 0\}$$

- Incurs no loss if the difference between the prediction and the target $\left|y_i - \mathbf{w}^\top \mathbf{x}^{(i)}\right|$ is less than ϵ