KYOTO UNIVERSITY

Statistical Learning Theory
- Classification -

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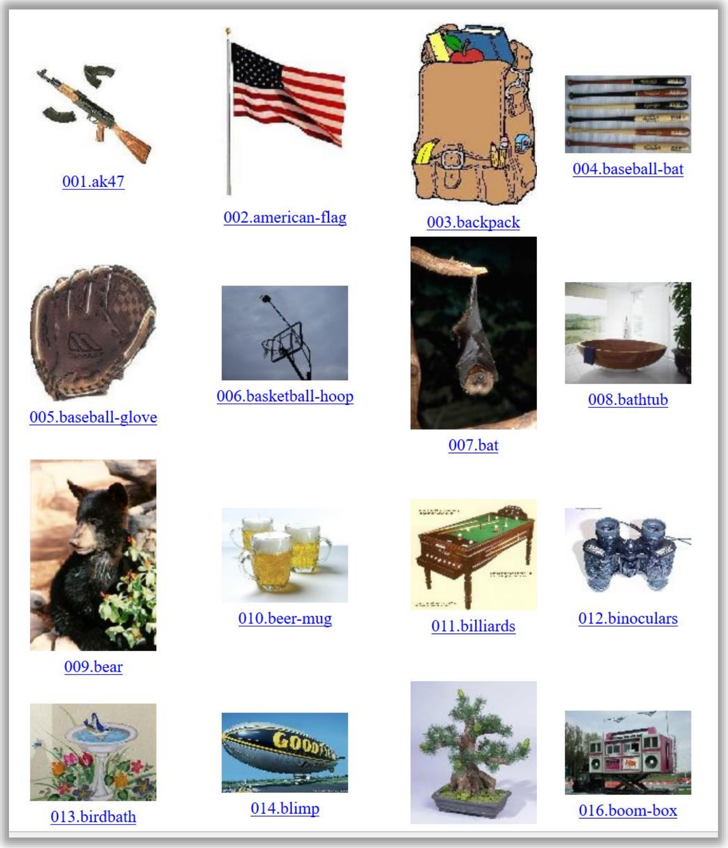
Classification

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 $\{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)})\}$



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

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

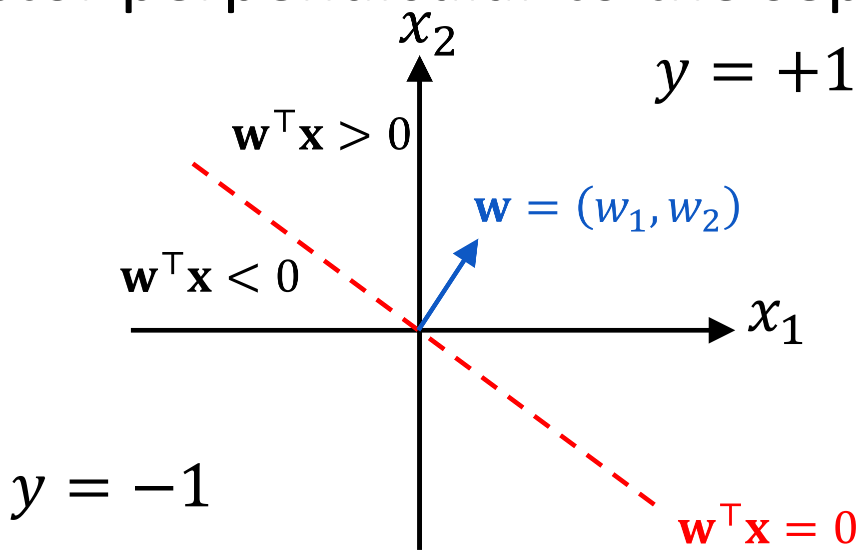
- Binary (two-class)classification:
  - Purchase prediction: Predict if a customer $\mathbf{x}$ will buy a particular product $(+1)$ or not (-1)
  - Credit risk prediction: Predict if a obligor $\mathbf{x}$ will pay back a debt $(+1)$ or not (-1)
- Multi-class classification ($\neq$ Multi-label classification):
  - 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 classification: Linear 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 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 : $\begin{cases} \text{Loss = Probabilistic model} \\ \text{Regularization = Prior} \end{cases}$

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

- Minimization problem: $\mathbf{w}^* = \operatorname{argmin}_{\mathbf{w}} L(\mathbf{w}) + R(\mathbf{w})$
  - 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:

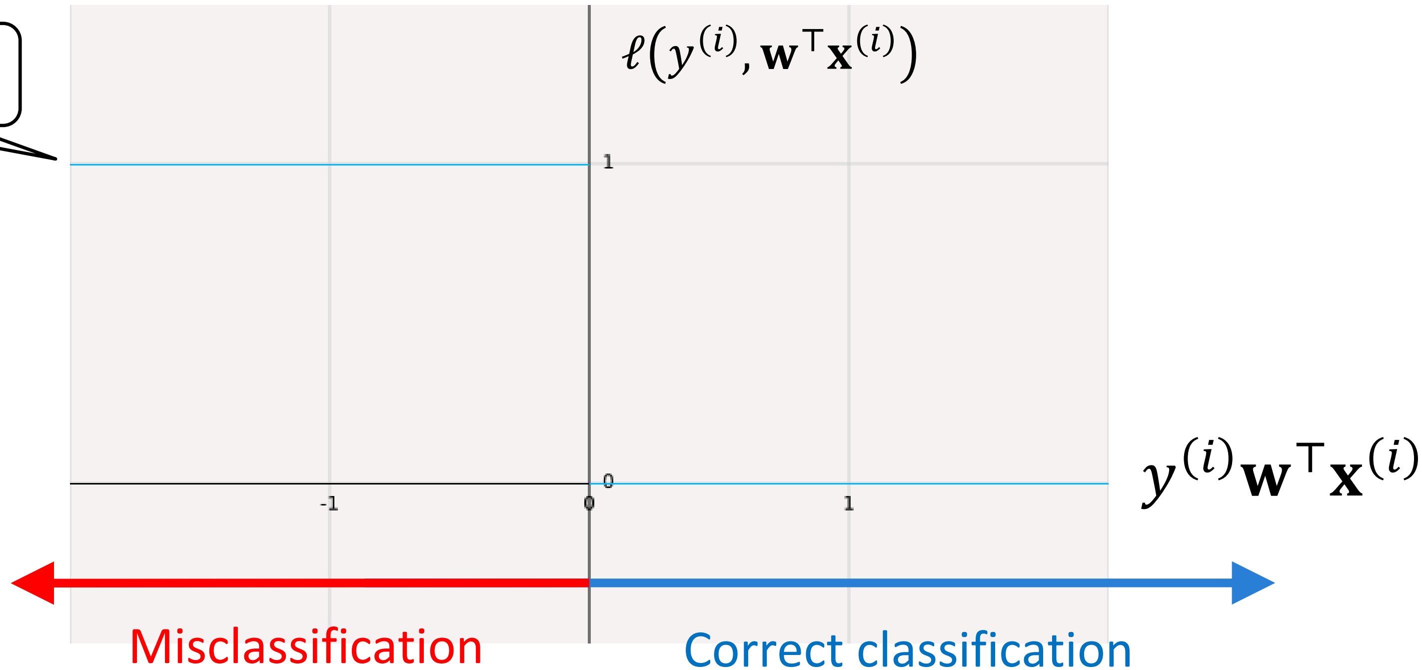
$$\ell^{(i)}\left(y^{(i)}, \mathbf{w}^\top \mathbf{x}^{(i)}\right) = \begin{cases} 0 & \left(y^{(i)} \underbrace{=}_{\text{Correct classification}} \operatorname{sign}\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) \\ 1 & \left(y^{(i)} \underbrace{\neq}_{\text{Incorrect classification}} \operatorname{sign}\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) \end{cases}$$

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

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

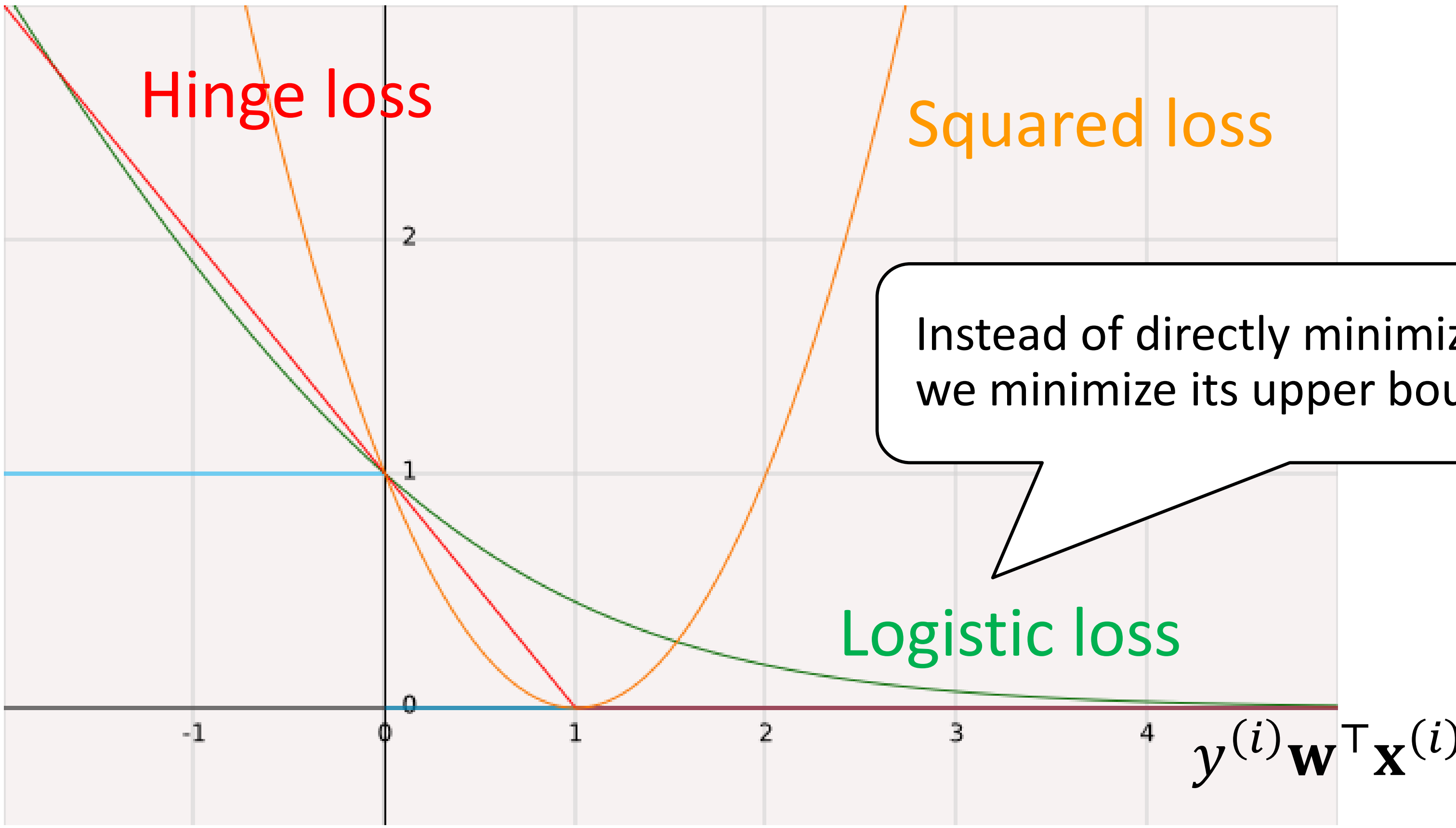
- Non-convex function is hard to optimize directly

Non-convex



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, ...



Instead of directly minimizing zero-one loss, we minimize its upper bound

Logistic regression

Logistic regression:
Minimization of logistic loss is a convex optimization

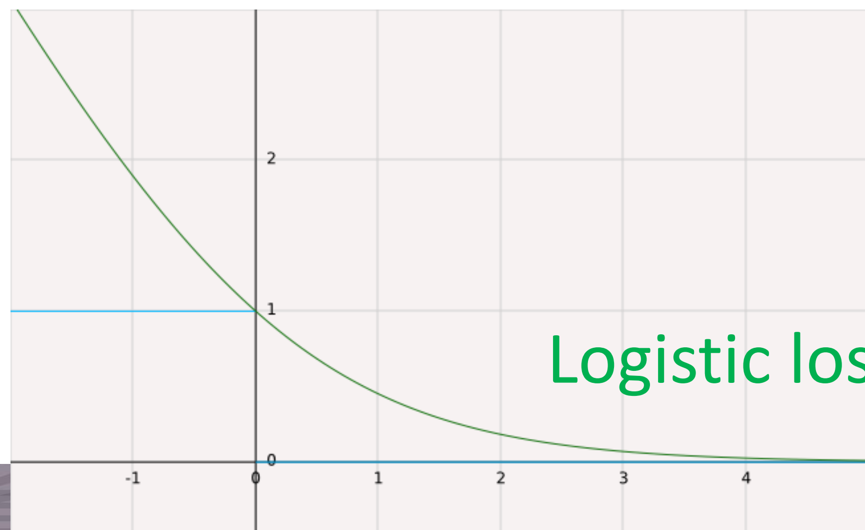
- Logistic loss:

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

- (Regularized) Logistic regression:

Convex

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



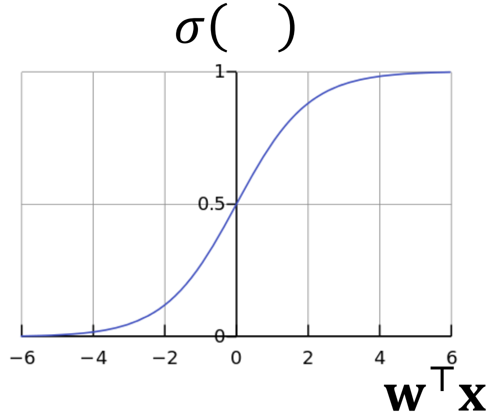
Statistical interpretation: Logistic loss min. as MLE of logistic regression model

- 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:

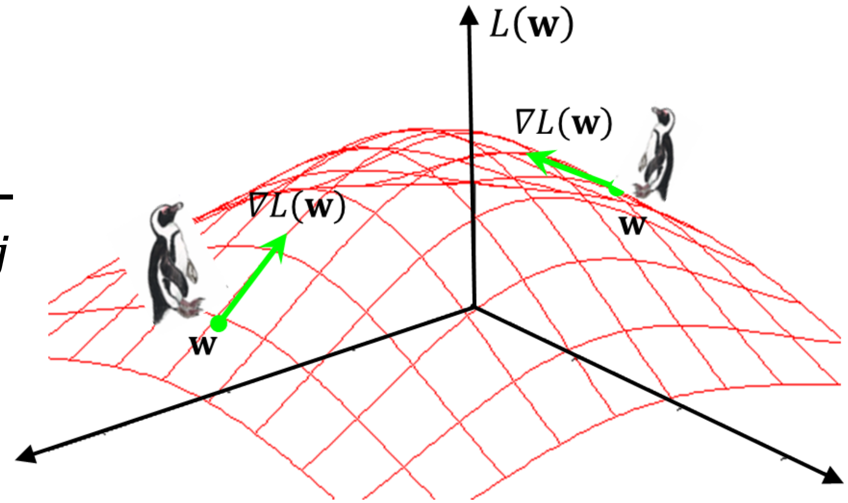
3rd-order term

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

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

  - Steepest direction

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



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:

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

$$\mathbf{w} \xrightarrow{-\boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})} \mathbf{w} - \boldsymbol{H}(\mathbf{w})^{-1}\nabla L(\mathbf{w})$$

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 $\boldsymbol{I}$ 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

$$\mathbf{w} \xrightarrow{-\eta \nabla L(\mathbf{w})} \mathbf{w} - \eta \nabla L(\mathbf{w})$$

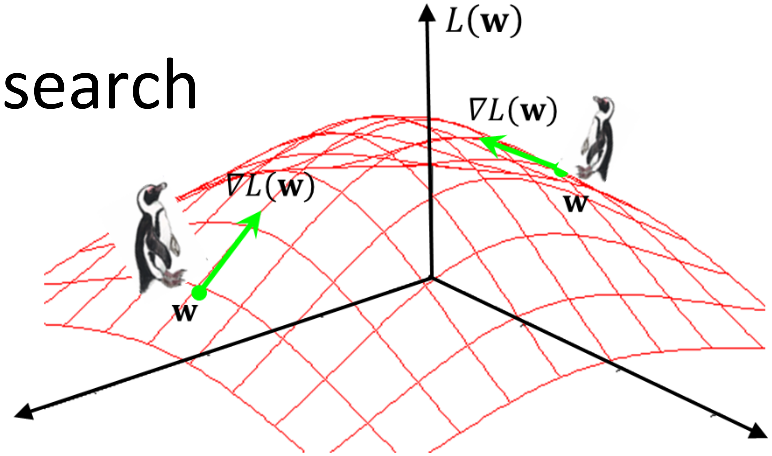
[Review]:
Gradient descent

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

– Learning rate η is determined by line search



Gradient of logistic regression:
Gradient descent of

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

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

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

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

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)

Support Vector Machine and Kernel Methods

Support vector machine (SVM): 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
  - Derived in accordance with the “maximum margin principle”
  - Understood as hinge loss + L2-regularization
- 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

1. "Soft-margin" SVM: hinge-loss + L2 regularization

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

– This is a convex optimization problem ☺

2. "Hard-margin": constraint on the loss (to be zero)

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

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

– The originally proposed SVM formulation was in this form

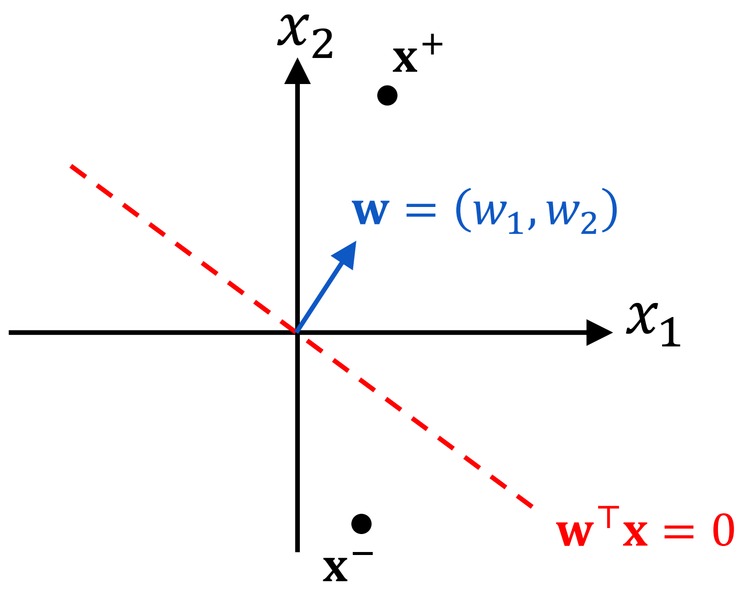
Geometric interpretation: Hard-margin SVM maximizes the margin

- $\min \frac{1}{2} \| \mathbf{w} \|_2^2 \leftrightarrow \max \frac{1}{\|\mathbf{w}\|_2}$ ($\frac{1}{\|\mathbf{w}\|_2}$ is called *margin*)

- $\frac{\mathbf{w}^\top(\mathbf{x}^+ - \mathbf{x}^-)}{\|\mathbf{w}\|_2}$: Sum of distance from separating hyperplane to a positive instance $\mathbf{x}^+$ and the distance to a negative instance $\mathbf{x}^-$

- Margin is the minimum of $\frac{\mathbf{w}^\top(\mathbf{x}^+ - \mathbf{x}^-)}{\|\mathbf{w}\|_2}$
  - Since $1 - y^{(i)}\mathbf{w}^\top\mathbf{x}^{(i)} \leq 0$ for $\forall i$,

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



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

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

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

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

  – 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 $1 - y^{(i)} \mathbf{w}^\top \mathbf{x}^{(i)} \le 0$ 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:

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

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

- Support vectors: 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 contribute to 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:
A similar dual problem with 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)

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

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

- Results in a similar dual problem with additional constraints:

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

$$0 \leq \alpha_i \leq C \quad (i = 1, 2, \ldots, N)$$

An important fact about SVM: Data access through inner products between data

- The dual form objective function and the classifier access to data always through inner products $\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$
  - Optimization problem (dual form):

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

  - Model : $y = \sum_{j=1}^{N} \alpha_j y^{(j)} \mathbf{x}^{(i)\top}\mathbf{x}$
  - The inner product $\mathbf{x}^{(i)\top}\mathbf{x}^{(j)}$ is interpreted as similarity

Kernel methods: Data access through kernel function

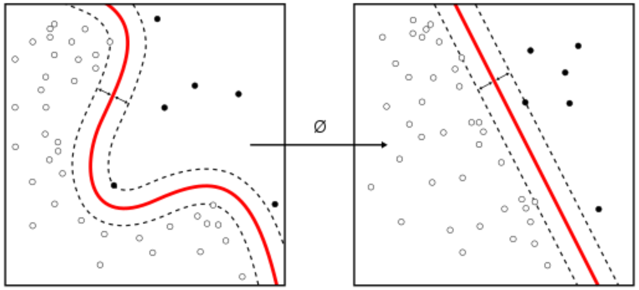
- The dual form objective function and the classifier access to data always through inner products ${\mathbf{x}^{(i)}}^\top \mathbf{x}^{(j)}$
- The inner product ${\mathbf{x}^{(i)}}^\top \mathbf{x}^{(j)}$ is interpreted as similarity
- Can we use some similarity function $K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)$ 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 $K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right)^{\top} \boldsymbol{\phi}(\mathbf{x}^{(j)})$ in the D'-dimensional space
- SVM is a linear classifier in the D'-dimensional space, while is a non-linear classifier in the original D-dimensional space



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

Advantage of kernel methods: Computationally efficient (when D' is large)

- Advantage of using kernel function

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

- Usually we expect the computation cost of K depends on D'
  - D' can be high-dimensional (possibly infinite dimensional)
- If we can somehow compute $\boldsymbol{\phi}\left(\mathbf{x}^{(i)}\right)^\top \boldsymbol{\phi}\left(\mathbf{x}^{(j)}\right)$ in time depending on D, the dimension of $\boldsymbol{\phi}$ does not matter
- Problem size:

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

  - Advantageous when D' is very large or infinite

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

- Combinatorial features: Not only the original features $x_1, x_2, \ldots, x_D$, we use their cross terms (e.g. $x_1 x_2$)
  - If we consider M-th order cross terms, we have $\mathrm{O}\left(D^M\right)$ terms

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

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

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

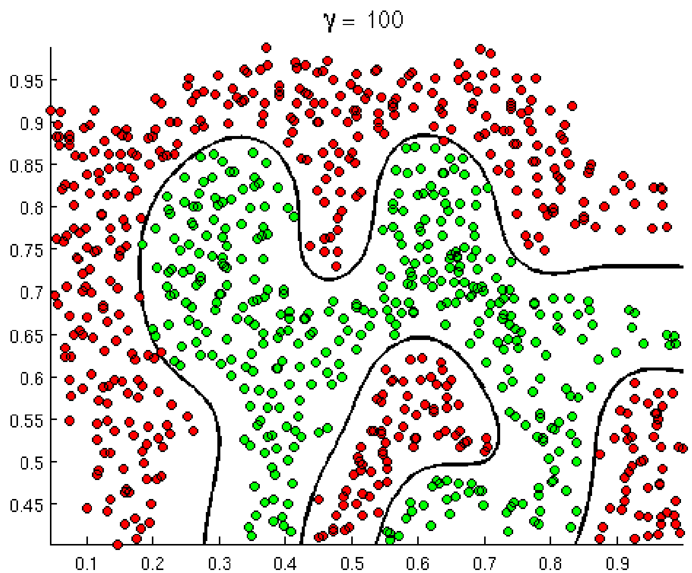
$$= \left({x_1^{(i)}}^2, {x_2^{(i)}}^2, \sqrt{2} x_1^{(i)} x_2^{(i)}\right)\left({x_1^{(j)}}^2, {x_2^{(j)}}^2, \sqrt{2} x_1^{(j)} x_2^{(j)}\right)$$

  - Note that it can be computed in $\mathrm{O}(D)$

Example of kernel functions: Gaussian kernel with infinite feature space

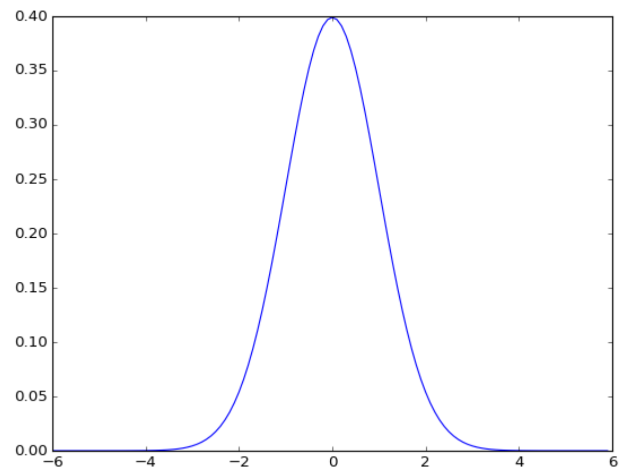
- Gaussian kernel (RBF kernel): $K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma}\right)$
  - Can be interpreted as an inner product in an infinite-dimensional space

Discrimination surface with Gaussian kernel



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

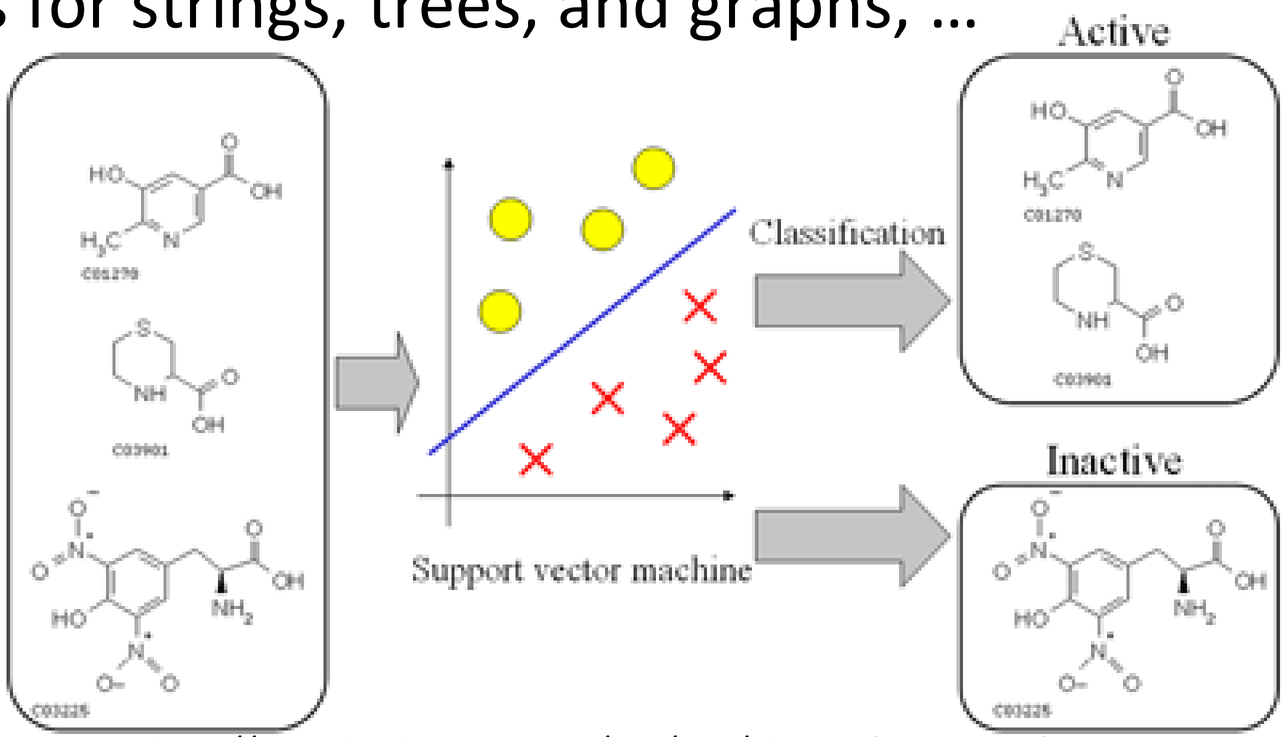
Gaussian kernel (RBF kernel)



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

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 functions are 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 classifier

$$\mathrm{sign}(\mathbf{w}^\top \mathbf{x}) = \mathrm{sign}\left(\sum_{j=1}^{N} \alpha_j y^{(j)} {\mathbf{x}^{(j)}}^\top \mathbf{x}\right)$$

- Representer theorem guarantees this (if we use L2-regularizer)

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

- Assumption: Loss ℓ for i-th data depends only on $\mathbf{w}^\top \mathbf{x}^{(i)}$
  - Objective function: $L(\mathbf{w}) = \sum_{i=1}^{N} \ell\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right) + \lambda \|\mathbf{w}\|_2^2$
- 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 $\left\{\mathbf{x}^{(i)}\right\}$)
- $L(\mathbf{w}^*)$ depends only on $\mathbf{w}$: $\sum_{i=1}^{N} \ell\left(\mathbf{w}^{*\top} \mathbf{x}^{(i)}\right) + \lambda \|\mathbf{w}^*\|_2^2$

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

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 zero loss if the difference between the prediction and the target $\left|y_i - \mathbf{w}^\top \mathbf{x}^{(i)}\right|$ is less than $\epsilon > 0$