# Introduction to Statistical Learning and Machine Learning

## Chap 5 & Chap6 – SVM and Kernel Methods

Yanwei Fu

School of Data Science, Fudan University

1. Recap of SVM and how to do the optimisation of SVM
2. Advanced issues of Dual form and Kernels of SVM
3. Appendix–Practical Issues in Machine Learning Experiments

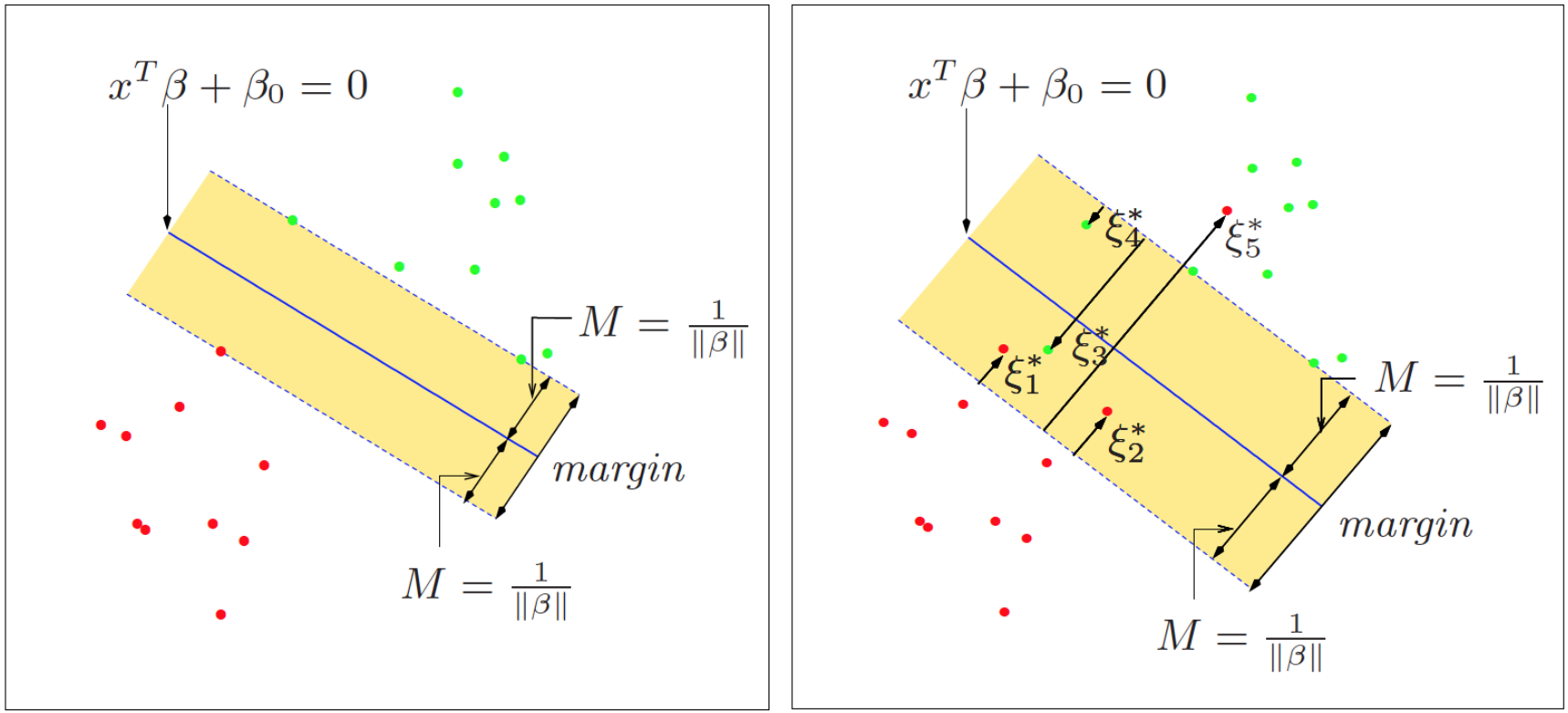



**FIGURE 12.1.** *Support vector classifiers. The left panel shows the separable case. The decision boundary is the solid line, while broken lines bound the shaded maximal margin of width* $2M = 2/\|\beta\|$. *The right panel shows the nonseparable (overlap) case. The points labeled* $\xi_j^*$ *are on the wrong side of their margin by an amount* $\xi_j^* = M\xi_j$; *points on the correct side have* $\xi_j^* = 0$. *The margin is maximized subject to a total budget* $\sum \xi_i \leq$ *constant. Hence* $\sum \xi_j^*$ *is the total distance of points on the wrong side of their margin.*

# Different Forms of SVM (seperated cases)

$$\max_{\beta,\beta_0,\|\beta\|_2=1} M$$
$$s.t. y_i\left(x_i^T\beta+\beta_0\right)\geqslant M,\quad i=1,\cdots,n \qquad (1)$$

which is equivalent to

$$\min \| \beta \|_2$$
$$s.t. y_i\left(x_i^T\beta+\beta_0\right)\geqq 1,\quad i=1,\cdots,n$$

A natural way to modify the constraint in Eq(1) is by introducing the slack variable $\xi=(\xi_1,\cdots,\xi_n)$:

$$y_i\left(x_i^T\beta+\beta_0\right)\geqslant M(1-\xi_i)$$

$\forall i,\xi_i\geqslant 0,\sum_i\xi_i\leqslant constant$
Remark: $M\sum_i\xi_i$ measures the total amount distance of points on the wrong side of their margin.

# Different Forms of SVM (non-seperatable cases)

$$\begin{aligned} &\min \| \beta \|_2^2 \\ &s.t. y_i \left( x_i^T \beta + \beta_0 \right) \geqslant 1 - \xi_i, \quad i = 1, \cdots, n \\ &\xi_i \geqslant 0, \sum_i \xi_i \leqslant constant \end{aligned} \tag{2}$$

$$\begin{aligned} &\min \frac{1}{2} \| \beta \|_2^2 + C \sum_i \xi_i \\ &s.t. y_i \left( x_i^T \beta + \beta_0 \right) \geqslant 1 - \xi_i, \quad i = 1, \cdots, n, \xi_i \geqslant 0 \end{aligned} \tag{3}$$

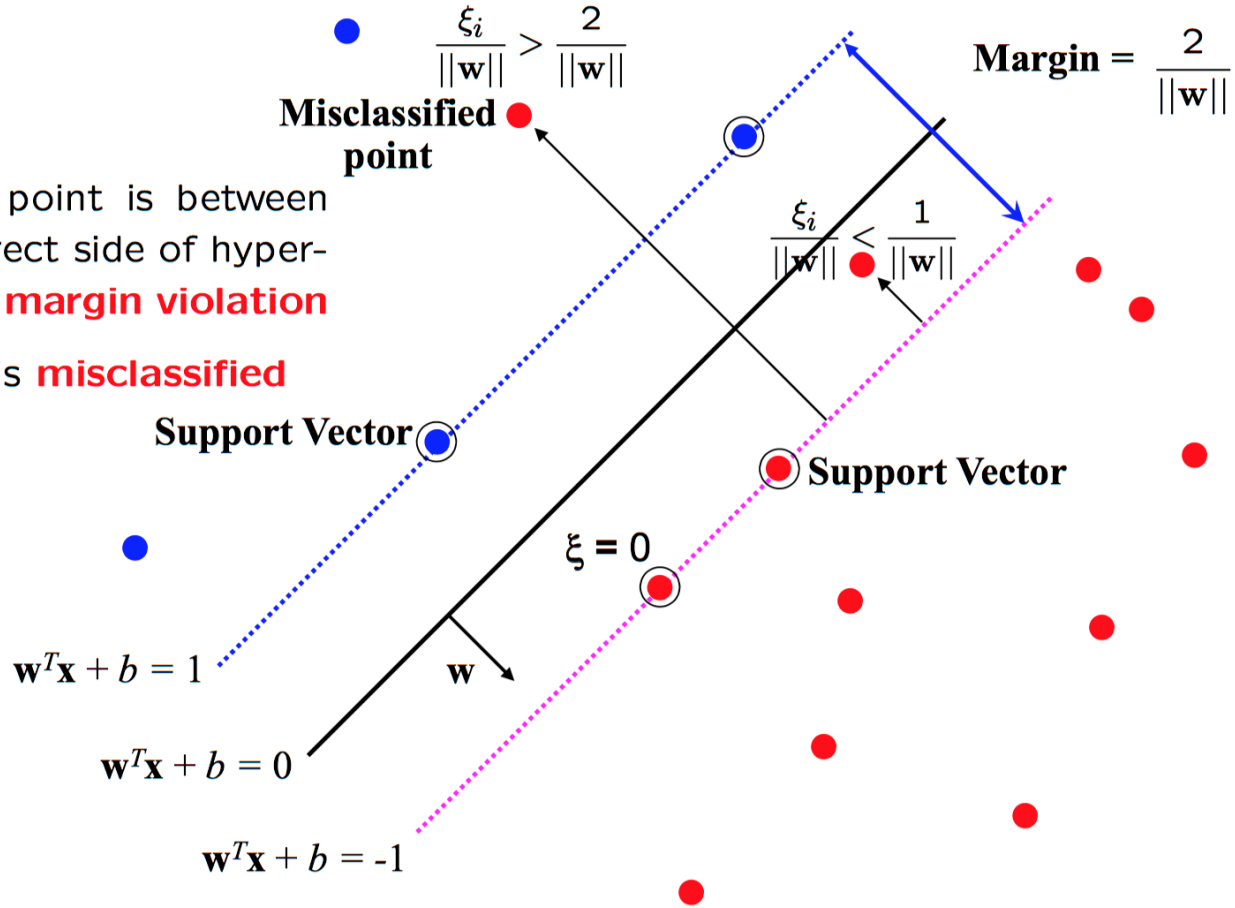
$$\min \sum_{i=1}^{n} \left[ 1 - y_i \left( x_i^T \beta + \beta_0 \right) \right]_+ + \frac{\lambda}{2} \| \beta \|_2^2 \tag{4}$$

where $x_+$ indicates the positive part of $x$. If $\lambda = C/2$, then Eq(3) and Eq(4) are equivalent.

# Introduce "slack" variables

$$\xi_i \geq 0$$

- for $0 < \xi \leq 1$ point is between margin and correct side of hyper-plane. This is a **margin violation**
- for $\xi > 1$ point is **misclassified**



Learning an SVM has been formulated as a constrained optimization problem over $\mathbf{w}$ and $\xi$

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i \text{ subject to } y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\dots N$$

The constraint $y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i$, can be written more concisely as

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with $\xi_i \geq 0$, is equivalent to

$$\xi_i = \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

Hence the learning problem is equivalent to the unconstrained optimization problem over $\mathbf{w}$

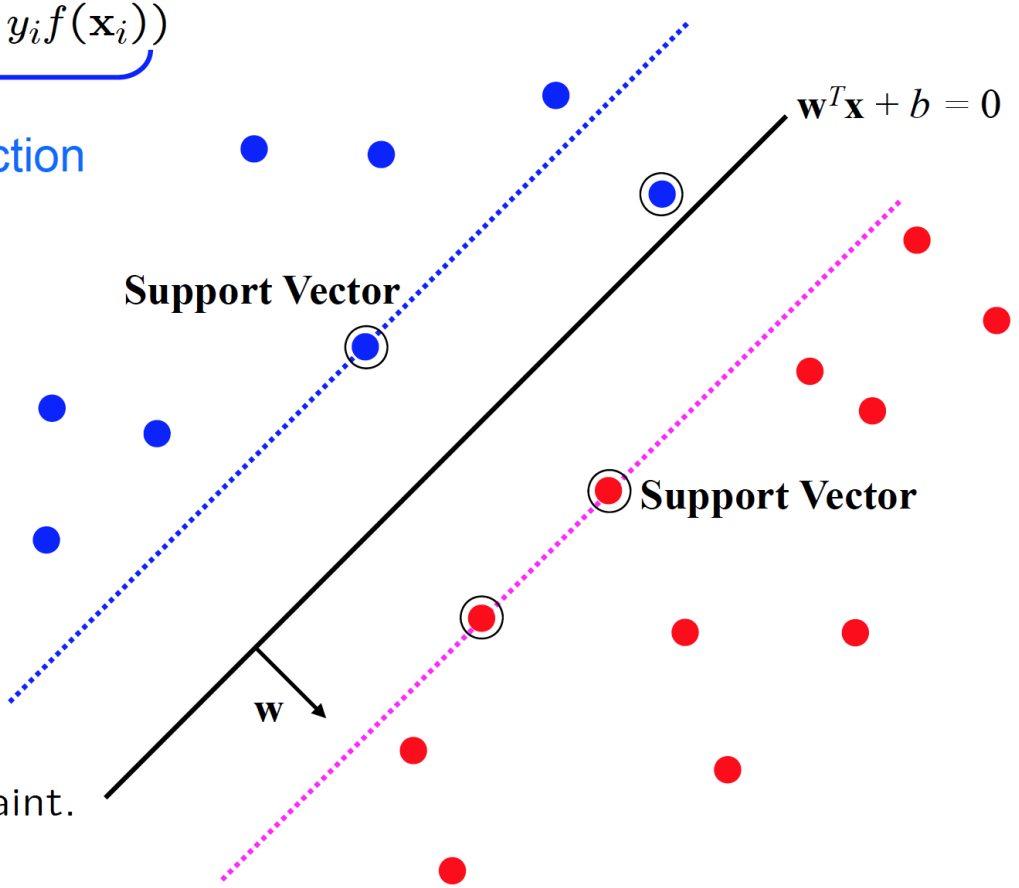
$$\min_{\mathbf{w}\in\mathbb{R}^d} \underbrace{||\mathbf{w}||^2}_{\text{regularization}} + C\sum_i^N \underbrace{\max\left(0, 1 - y_i f(\mathbf{x}_i)\right)}_{\text{loss function}}$$

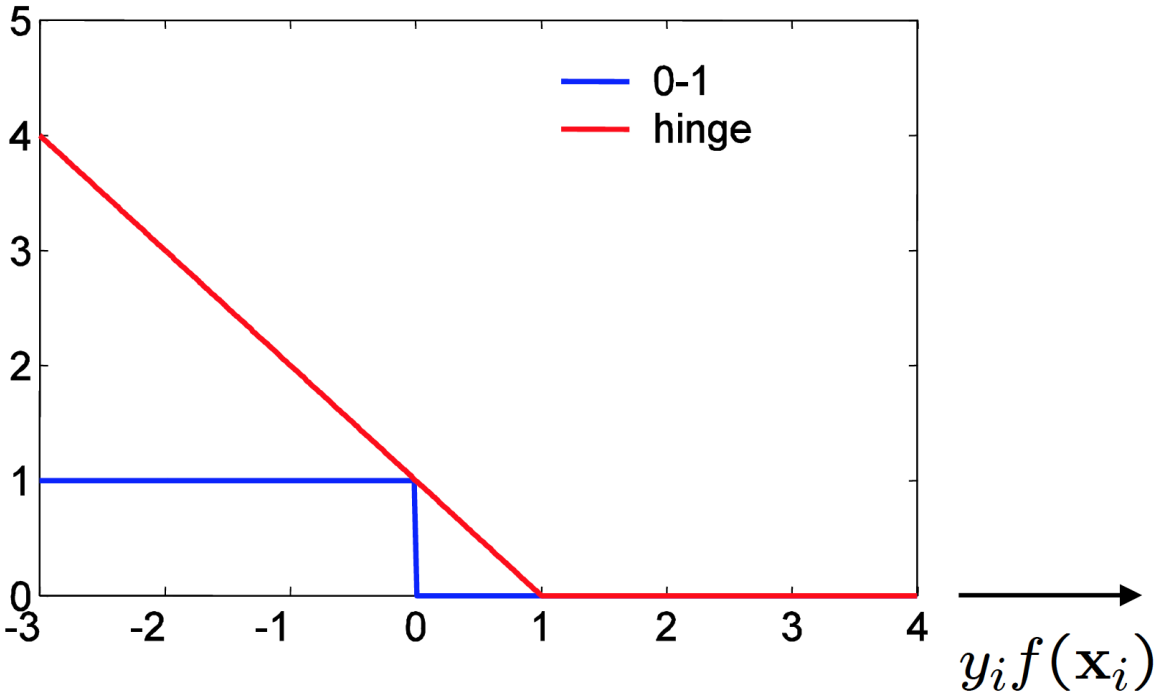
# Loss function

$$\min_{\mathbf{w}\in\mathbb{R}^d} ||\mathbf{w}||^2 + C\sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

Points are in three categories:

1. $y_i f(x_i) > 1$
   Point is outside margin.
   No contribution to loss
2. $y_i f(x_i) = 1$
   Point is on margin.
   No contribution to loss.
   As in hard margin case.
3. $y_i f(x_i) < 1$
   Point violates margin constraint.
   Contributes to loss

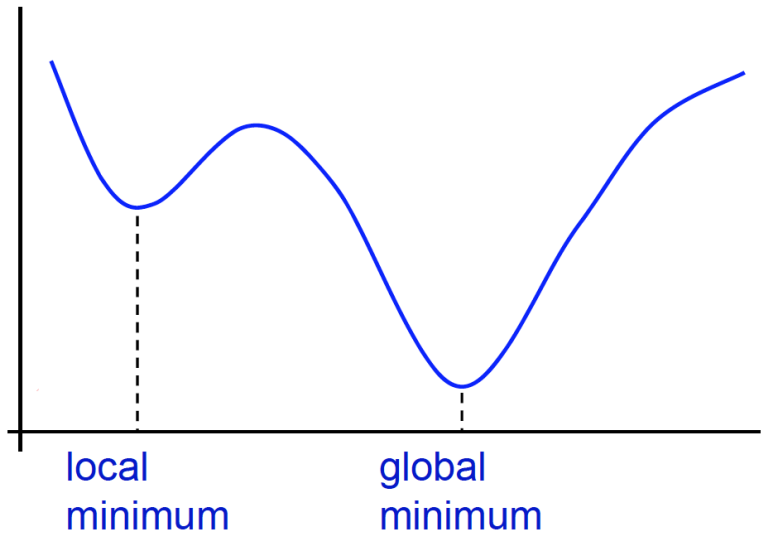





- SVM uses "hinge" loss $\max(0, 1 - y_i f(x_i))$
- an approximation to the 0-1 loss

# Optimization continued

$$\min_{\mathbf{w}\in\mathbb{R}^d} C\sum_{i}^{N}\max\left(0,1-y_i f(\mathbf{x}_i)\right)+||\mathbf{w}||^2$$

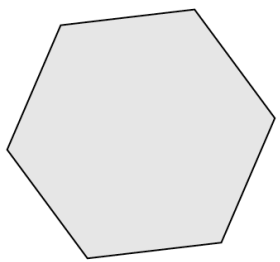



- Does this cost function have a unique solution?
- Does the solution depend on the starting point of an iterative optimization algorithm (such as gradient descent)?

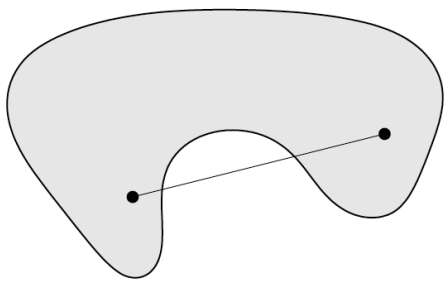
If the cost function is convex, then a locally optimal point is globally optimal (provided the optimization is over a convex set, which it is in our case)

contains the line segment between any two points in the set

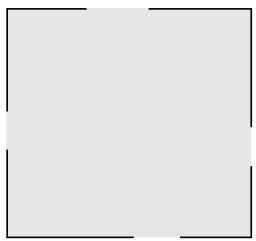
$$x_1, x_2 \in C, \quad 0 \leq \theta \leq 1 \quad \Longrightarrow \quad \theta x_1 + (1-\theta)x_2 \in C$$



convex



not convex



not convex

**Affine set:** solution set of linear equations $Ax = b$

**Halfspace:** solution of one linear inequality $a^T x \leq b$ $(a \neq 0)$

**Polyhedron:** solution of finitely many linear inequalities $Ax \leq b$

**Ellipsoid:** solution of positive definite quadratic inequality

$$(x - x_c)^T A(x - x_c) \leq 1 \qquad (A \text{ positive definite})$$

**Norm ball:** solution of $\|x\| \leq R$ (for any norm)

**Positive semidefinite cone:** $\mathbf{S}_+^n = \{X \in \mathbf{S}^n \mid X \succeq 0\}$

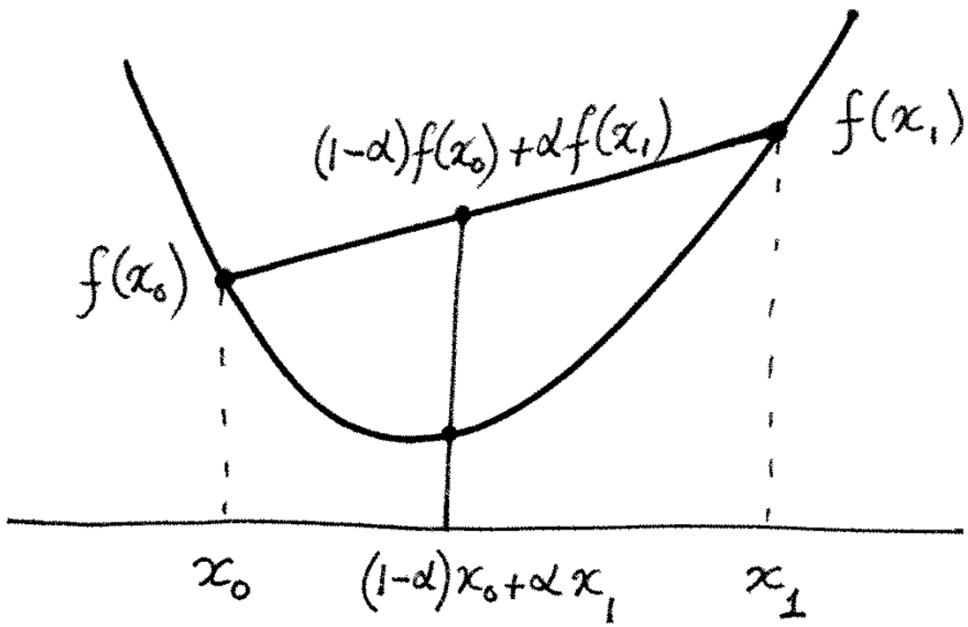
the **intersection** of any number of convex sets is convex

$D$ – a domain in $\mathbb{R}^n$.

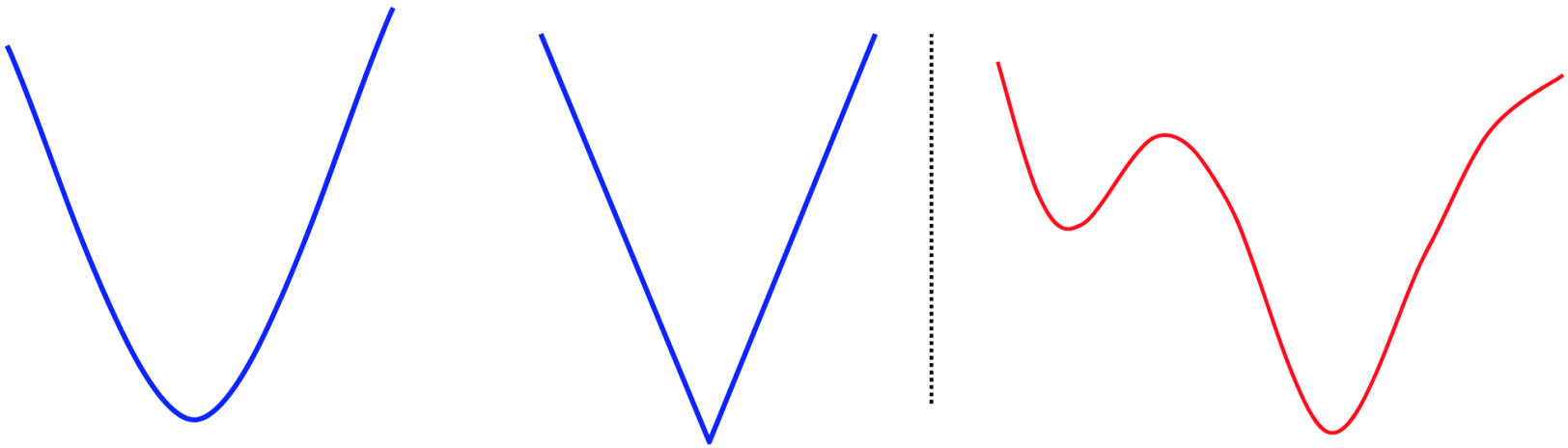
A convex function $f : D \to \mathbb{R}$ is one that satisfies, for any $\mathbf{x}_0$ and $\mathbf{x}_1$ in $D$:

$$f((1-\alpha)\mathbf{x}_0 + \alpha\mathbf{x}_1) \leq (1-\alpha)f(\mathbf{x}_0) + \alpha f(\mathbf{x}_1) \ .$$

Line joining $(\mathbf{x}_0, f(\mathbf{x}_0))$ and $(\mathbf{x}_1, f(\mathbf{x}_1))$ lies above the function graph.



# Convex function examples

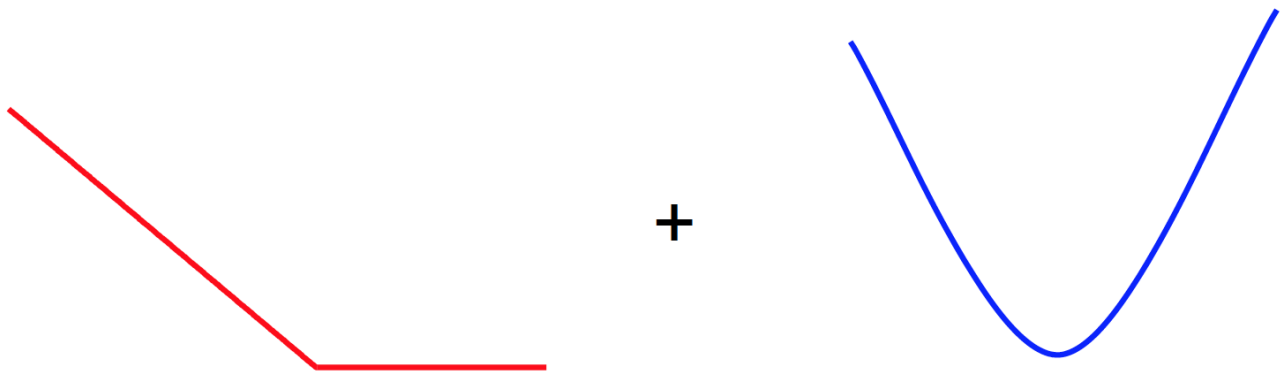



A non-negative sum of convex functions is convex

# More examples

- linear and affine functions are convex and concave
- $\exp x$, $-\log x$, $x \log x$ are convex
- $x^\alpha$ is convex for $x > 0$ and $\alpha \geq 1$ or $\alpha \leq 0$; $|x|^\alpha$ is convex for $\alpha \geq 1$
- norms are convex
- quadratic-over-linear function $x^T x/t$ is convex in $x$, $t$ for $t > 0$
- geometric mean $(x_1 x_2 \cdots x_n)^{1/n}$ is concave for $x \geq 0$
- $\log \det X$ is concave on set of positive definite matrices
- $\log(e^{x_1} + \cdots e^{x_n})$ is convex

# As for SVM, we have ...



SVM

$$\min_{\mathbf{w}\in\mathbb{R}^d} C\sum_{i}^{N}\max\left(0,1-y_i f(\mathbf{x}_i)\right)+||\mathbf{w}||^2$$

convex

# Gradient (or steepest) descent algorithm for SVM

To minimize a cost function $\mathcal{C}(\mathbf{w})$ use the iterative update

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla_{\mathbf{w}} \mathcal{C}(\mathbf{w}_t)$$

where $\eta$ is the learning rate.

First, rewrite the optimization problem as an average

$$\begin{aligned} \min_{\mathbf{w}} \mathcal{C}(\mathbf{w}) &= \frac{\lambda}{2}||\mathbf{w}||^2 + \frac{1}{N}\sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i)) \\ &= \frac{1}{N}\sum_i^N \left(\frac{\lambda}{2}||\mathbf{w}||^2 + \max(0, 1 - y_i f(\mathbf{x}_i))\right) \end{aligned}$$

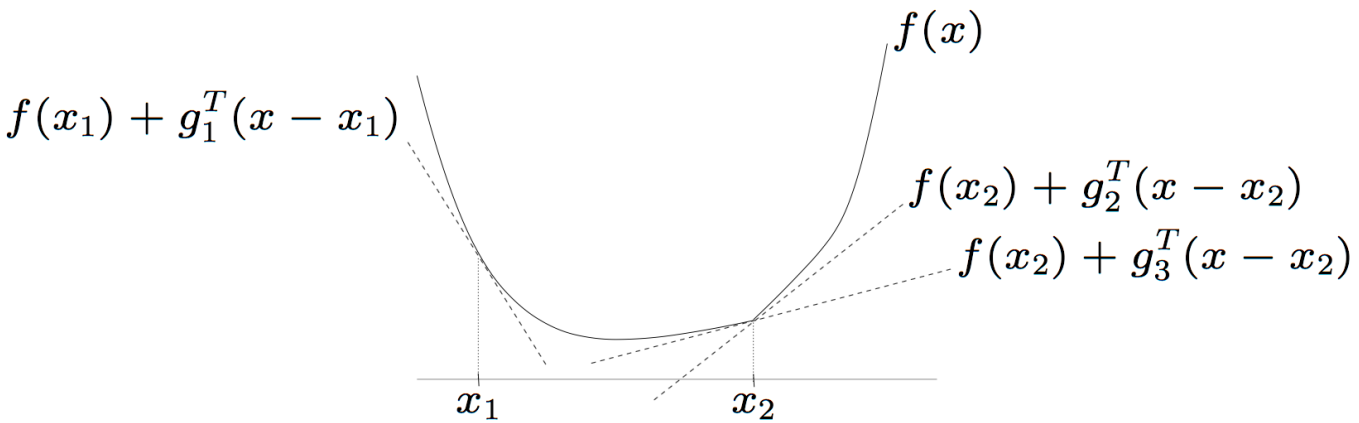
(with $\lambda = 2/(NC)$ up to an overall scale of the problem) and $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

Because the hinge loss is not differentiable, a sub-gradient is computed

$g$ is a **subgradient** of $f$ (not necessarily convex) at $x$ if

$$f(y) \geq f(x) + g^T(y - x) \quad \text{for all } y$$

($\iff (g, -1)$ supports $\mathbf{epi}\, f$ at $(x, f(x))$)

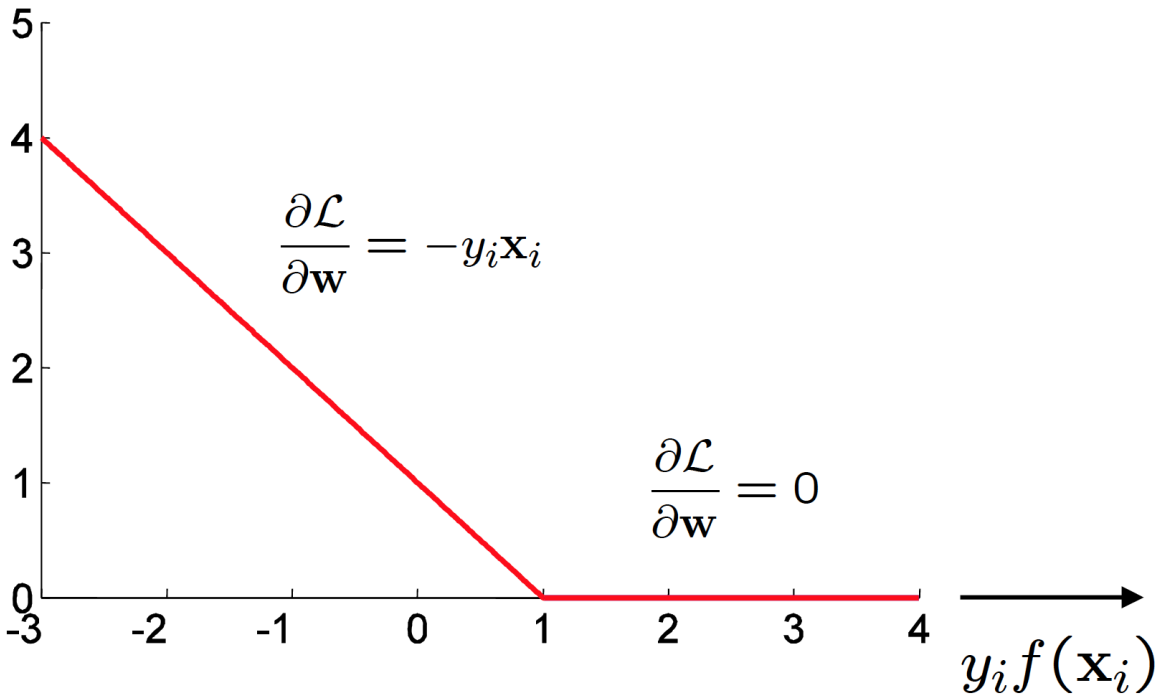



$g_2$, $g_3$ are subgradients at $x_2$; $g_1$ is a subgradient at $x_1$

Prof. S. Boyd, EE392o, Stanford University

# Sub-gradient for hinge loss

$$\mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}) = \max(0, 1 - y_i f(\mathbf{x}_i)) \qquad f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + b$$



# Sub-gradient descent algorithm for SVM

$$\mathcal{C}(\mathbf{w}) = \frac{1}{N}\sum_{i}^{N}\left(\frac{\lambda}{2}||\mathbf{w}||^2 + \mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w})\right)$$

The iterative update is

$$\begin{aligned}\mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta\nabla_{\mathbf{w}_t}\mathcal{C}(\mathbf{w}_t) \\ &\leftarrow \mathbf{w}_t - \eta\frac{1}{N}\sum_{i}^{N}(\lambda\mathbf{w}_t + \nabla_{\mathbf{w}}\mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}_t))\end{aligned}$$

where $\eta$ is the learning rate.

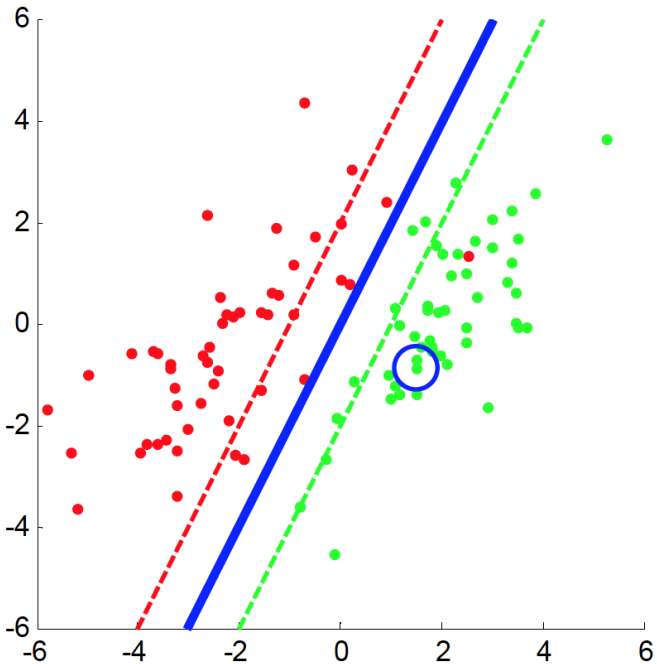
Then each iteration $t$ involves cycling through the training data with the updates:

$$\begin{aligned}\mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta(\lambda\mathbf{w}_t - y_i\mathbf{x}_i) \qquad \text{if } y_i f(\mathbf{x}_i) < 1 \\ &\leftarrow \mathbf{w}_t - \eta\lambda\mathbf{w}_t \qquad \text{otherwise}\end{aligned}$$

In the Pegasos algorithm the learning rate is set at $\eta_t = \frac{1}{\lambda t}$

# Pegasos – Stochastic Gradient Descent Algorithm

## Randomly sample from the training data


Pegasos: Primal Estimated sub-GrAdient SOlver for SVM (ICML 2007)

Advanced issues of Dual form and Kernels of SVM
Detailed duality, please refer to Page 215 – 229, (Chap 5), Stephen Byod et al. “Convex Optimization” 2004, Cambridge University Press

# Dual Form of SVM

- We have seen that for an SVM learning a linear classifier

$$f(x) = \mathbf{w}^\top \mathbf{x} + b$$

is formulated as solving an optimization problem over $\mathbf{w}$ :

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i))$$

- This quadratic optimization problem is known as the primal problem.

- Instead, the SVM can be formulated to learn a linear classifier

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

by solving an optimization problem over $\alpha_i$.

- This is know as the dual problem, and we will look at the advantages of this formulation.

# Sketch derivation of dual form

The Representer Theorem states that the solution $\mathbf{w}$ can always be written as a linear combination of the training data:

$$\mathbf{w} = \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j$$

Now, substitute for $\mathbf{w}$ in $f(x) = \mathbf{w}^\top \mathbf{x} + b$

$$f(x) = \left( \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \right)^\top \mathbf{x} + b = \sum_{j=1}^{N} \alpha_j y_j \left( \mathbf{x}_j{}^\top \mathbf{x} \right) + b$$

and for $\mathbf{w}$ in the cost function $\min_{\mathbf{w}} ||\mathbf{w}||^2$ subject to $y_i \left( \mathbf{w}^\top \mathbf{x}_i + b \right) \geq 1, \forall i$

$$||\mathbf{w}||^2 = \left\{ \sum_j \alpha_j y_j \mathbf{x}_j \right\}^\top \left\{ \sum_k \alpha_k y_k \mathbf{x}_k \right\} = \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k)$$

Hence, an equivalent optimization problem is over $\alpha_j$

$$\min_{\alpha_j} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \quad \text{subject to } y_i \left( \sum_{j=1}^{N} \alpha_j y_j (\mathbf{x}_j{}^\top \mathbf{x}_i) + b \right) \geq 1, \forall i$$

and a few more steps are required to complete the derivation.

# Primal and dual formulations (1)

$N$ is number of training points, and $d$ is dimension of feature vector $\mathbf{x}$.

Primal problem: for $\mathbf{w} \in \mathbb{R}^d$

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i))$$

Dual problem: for $\boldsymbol{\alpha} \in \mathbb{R}^N$ (stated without proof):

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \text{ subject to } 0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

- Need to learn $d$ parameters for primal, and $N$ for dual
- If $N << d$ then more efficient to solve for $\alpha$ than $\mathbf{w}$
- Dual form only involves $(\mathbf{x}_j{}^\top \mathbf{x}_k)$. We will return to why this is an advantage when we look at kernels.

# Primal and dual formulations (2)

Primal version of classifier:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

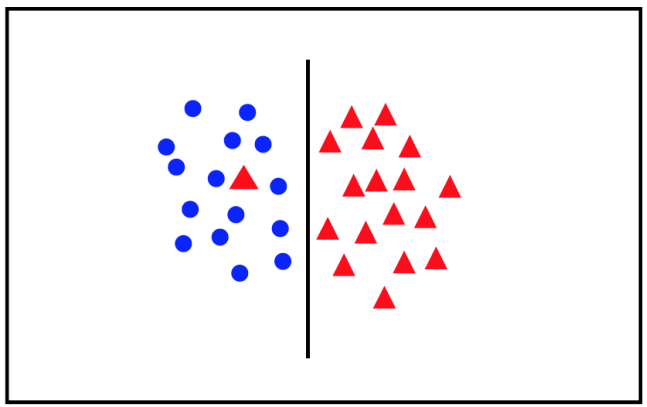
Dual version of classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

At first sight the dual form appears to have the disadvantage of a K-NN classifier – it requires the training data points $\mathbf{x}_i$. However, many of the $\alpha_i$'s are zero. The ones that are non-zero define the support vectors $\mathbf{x}_i$.

# Handling data that is not linearly separable

## motivation for introducing the dual form of SVM

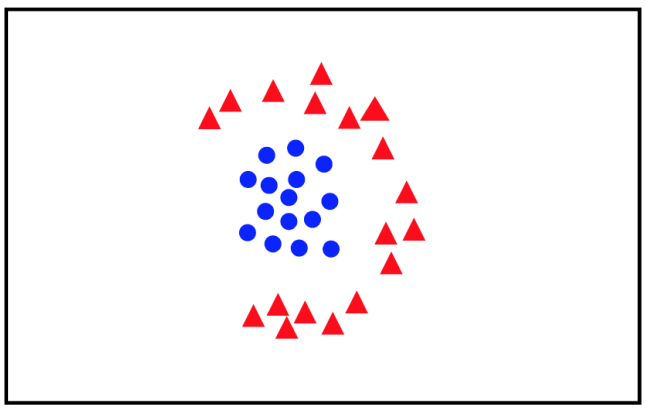


- introduce slack variables

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i$$

subject to

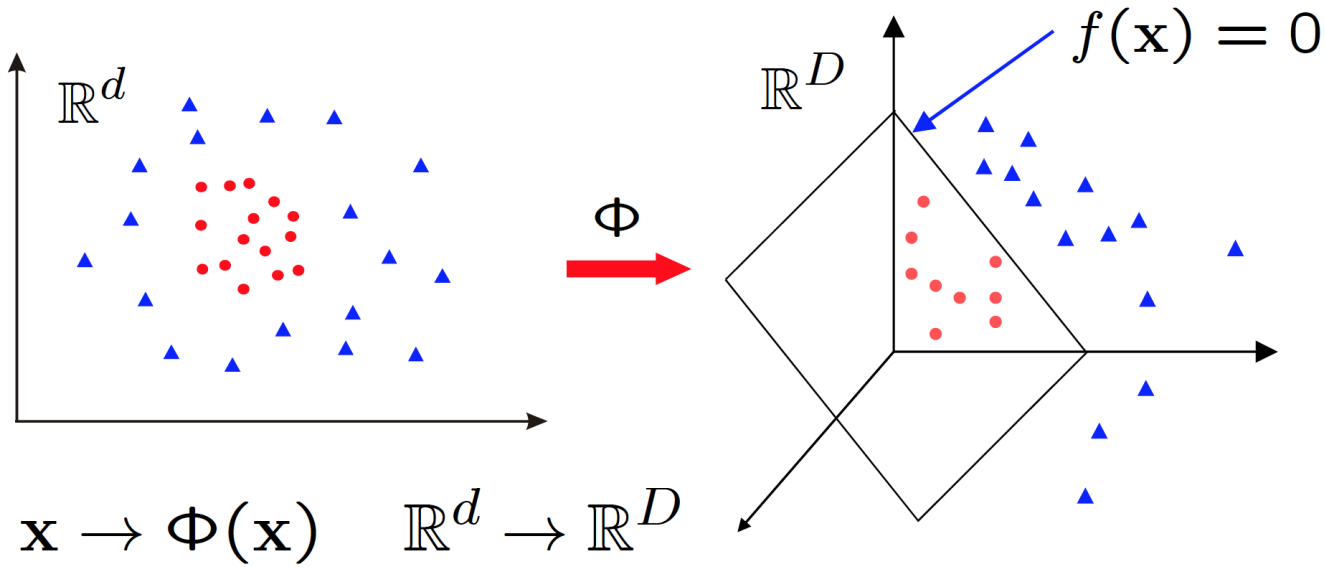
$$y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\ldots N$$



- linear classifier not appropriate

??

# SVM classifiers in a transformed feature space




$$\Phi : \mathbf{x} \to \Phi(\mathbf{x}) \quad \mathbb{R}^d \to \mathbb{R}^D$$

Learn classifier linear in $\mathbf{w}$ for $\mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

$\Phi(\mathbf{x})$ is a feature map

# Primal Classifier in transformed feature space

Classifier, with $\mathbf{w} \in \mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

Learning, for $\mathbf{w} \in \mathbb{R}^D$

$$\min_{\mathbf{w} \in \mathbb{R}^D} ||\mathbf{w}||^2 + C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i))$$

- Simply map $\mathbf{x}$ to $\Phi(\mathbf{x})$ where data is separable
- Solve for $\mathbf{w}$ in high dimensional space $\mathbb{R}^D$
- If $D >> d$ then there are many more parameters to learn for $\mathbf{w}$. Can this be avoided?

# Dual Classifier in transformed feature space

Classifier:

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \, \mathbf{x}_i{}^{\top} \mathbf{x} + b$$

$$\rightarrow f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \, \Phi(\mathbf{x}_i)^{\top} \Phi(\mathbf{x}) + b$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{x}_j{}^{\top} \mathbf{x}_k$$

$$\rightarrow \max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \Phi(\mathbf{x}_j)^{\top} \Phi(\mathbf{x}_k)$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

# Dual Classifier in transformed feature space

- Note, that $\Phi(\mathbf{x})$ only occurs in pairs $\Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$
- Once the scalar products are computed, only the $N$ dimensional vector $\boldsymbol{\alpha}$ needs to be learnt; it is not necessary to learn in the $D$ dimensional space, as it is for the primal
- Write $k(\mathbf{x}_j, \mathbf{x}_i) = \Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$. This is known as a Kernel

Classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \, k(\mathbf{x}_i, \mathbf{x}) + b$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \, k(\mathbf{x}_j, \mathbf{x}_k)$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \quad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$\begin{aligned} \Phi(\mathbf{x})^\top \Phi(\mathbf{z}) &= \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1z_2 \end{pmatrix} \\ &= x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2 \\ &= (x_1z_1 + x_2z_2)^2 \\ &= (\mathbf{x}^\top \mathbf{z})^2 \end{aligned}$$

## Kernel Trick

- Classifier can be learnt and applied without explicitly computing $\Phi(\mathbf{x})$
- All that is required is the kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$
- Complexity of learning depends on $N$

# Example kernels

- Linear kernels $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$
- Polynomial kernels $k(\mathbf{x}, \mathbf{x}') = \left(1 + \mathbf{x}^\top \mathbf{x}'\right)^d$ for any $d > 0$
  - Contains all polynomials terms up to degree $d$
- Gaussian kernels $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$ for $\sigma > 0$
  - Infinite dimensional feature space

N = size of training data

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$$

weight (may be zero)

support vector

Gaussian kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2/2\sigma^2\right)$

Radial Basis Function (RBF) SVM

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2/2\sigma^2\right) + b$$

# Constructing Kernels

Checking if a given function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel can be hard.

- $k(x, \bar{x}) = \tanh(1 + \langle x, \bar{x} \rangle)$ ?
- $k(x, \bar{x}) = \exp(\ -$ edit distance between two strings $x$ and $\bar{x}\ )$ ?
- $k(x, \bar{x}) = 1 - \|x - \bar{x}\|^2$ ?

Easier: construct functions that are garanteed to be kernels:

Construct explicitly:

- any $\phi : \mathcal{X} \to \mathbb{R}^m$ induces a kernel $k(x, \bar{x}) = \langle \phi(x), \phi(\bar{x}) \rangle$.
  in particular any $f : \mathcal{X} \to \mathbb{R}$, $\quad k(x, \bar{x}) = f(x) f(\bar{x})$

Construction from other kernels:

- If $k$ is a kernel and $\alpha \in \mathbb{R}^+$, then $k + \alpha$ and $\alpha k$ are kernels.
- if $k_1, k_2$ are kernels, then $k_1 + k_2$ and $k_1 \cdot k_2$ are kernels.
- if $k$ is a kernel, then $\exp(k)$ is a kernel.

# Appendix–Practical Issues in Machine Learning Experiments

# Optimizing the SVM Dual (kernelized)

How to solve the QP

$$\max_{\alpha^1,\ldots,\alpha^n \in \mathbb{R}} \quad -\frac{1}{2}\sum_{i,j=1}^{n} \alpha^i \alpha^j y^i y^j k(x^i, x^j) + \sum_{i=1}^{n} \alpha^i$$

subject to $\sum_i \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq C$, for $i = 1, \ldots, n$.

Observations:

- Kernel matrix $K$ (with entries $k_{ij} = k(x^i, x^j)$) might be too big to fit into memory.
- In the optimum, many of the $\alpha_i$ are $0$ and do not contribute. If we knew which ones, we would save a lot of work

# Optimizing the SVM Dual (kernelized)

**Working set training [Osuna 1997]**

1: $S = \emptyset$
2: **repeat**
3: $\alpha \leftarrow$ solve QP with variables $\alpha_i$ for $i \in S$ and $\alpha_i = 0$ for $i \notin S$
4: **for** $i = 1 \ldots, n$ **do**
5: **if** if $i \in S$ and $\alpha_i = 0$ **then** remove $i$ from $S$
6: **if** if $i \notin S$ and $\alpha_i$ not optimal **then** add $i$ to $S$
7: **end for**
8: **until** convergence

Advantages:

- objective value increases monotonously
- converges to global optimum

Disadvantages:

- each step is computationally costly, since $S$ can become large

## Sequential Minimal Optimization (SMO) [Platt 1998]

1: $\alpha \leftarrow 0$
2: **repeat**
3: pick index $i$ such that $\alpha_i$ is not optimal
4: pick index $j \neq i$ arbitrarily (usually based on some heuristic)
5: $\alpha_i, \alpha_j \leftarrow$ solve QP for $\alpha_i, \alpha_j$ and all other $\alpha_k$ fixed
6: **until** convergence

Advantages:

- convergences monotonously to global optimum
- each step optimizes a subproblem of smallest possible size: 2 unknowns (1 doesn't work because of constraint $\sum_i \alpha_i y_i = 0$)
- subproblems have a closed-form solution

Disadvantages:

- many iterations are required
- many kernel values $k(x^i, x^j)$ are computed more than once (unless $K$ is stored as matrix)

# SVMs Without Bias Term– Optimization

For optimization, the *bias term* is an annoyance

- In primal optimization, it often requires a different stepsize.
- In dual optimization, it is not straight-forward to recover.
- It couples the dual variables by an equality constraint: $\sum_i \alpha_i y_i = 0$.

We can get rid of the bias by the **augmentation trick**.

Original:

- $f(x) = \langle w, x \rangle_{\mathbb{R}^d} + b, \quad \text{with } w \in \mathbb{R}^d, b \in \mathbb{R}.$

New augmented:

- linear: $f(x) = \langle \tilde{w}, \tilde{x} \rangle_{\mathbb{R}^{d+1}}, \quad \text{with } \tilde{w} = (w, b),\ \tilde{x} = (x, 1).$
- generalized: $f(x) = \langle \tilde{w}, \tilde{\phi}(x) \rangle_{\tilde{\mathcal{H}}}$ with $\tilde{w} = (w, b),\ \tilde{\phi}(x) = (\phi(x), 1).$
- kernelize: $\tilde{k}(x, \bar{x}) = \langle \tilde{\phi}(x), \tilde{\phi}(\bar{x}) \rangle_{\tilde{\mathcal{H}}} = k(x, \bar{x}) + 1.$

# SVMs Without Bias Term– Optimization

**SVM without bias term – primal optimization problem**

$$\min_{w\in\mathbb{R}^d,\xi\in\mathbb{R}^n} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi^i$$

subject to, for $i = 1, \ldots, n$,

$$y^i\langle w, x^i\rangle \geq 1 - \xi^i, \qquad \text{and} \qquad \xi^i \geq 0.$$

Difference: no $b$ variable to optimize over

# SVMs Without Bias Term– Optimization

**SVM without bias term – primal optimization problem**

$$\min_{w\in\mathbb{R}^d,\xi\in\mathbb{R}^n} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi^i$$

subject to, for $i = 1,\ldots,n$,

$$y^i\langle w, x^i\rangle \geq 1-\xi^i, \qquad \text{and} \qquad \xi^i \geq 0.$$

Difference: no $b$ variable to optimize over

**SVM without bias term – dual optimization problem**

$$\max_{\alpha} \quad -\frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y^i y^j\, k(x^i,x^j) + \sum_i \alpha_i$$

subject to, $\quad 0 \leq \alpha_i \leq C, \quad$ for $i = 1,\ldots,n.$

Difference: no constraint $\sum_i y_i\alpha_i = 0$.

# Linear SVM Optimization in the Dual

**Stochastic Coordinate Dual Ascent**

$\alpha \leftarrow \mathbf{0}$.
**for** $t = 1, \ldots, T$ **do**
  $i \leftarrow$ random index (uniformly random or in epochs)
  solve QP w.r.t. $\alpha_i$ with all $\alpha_j$ for $j \neq i$ fixed.
**end for**
return $\alpha$

Properties:

- converges monotonically to global optimum
- each subproblem has smallest possible size

Open Problem:

- how to make each step efficient?

# SVM Optimization in the Dual

What's the complexity of the update step? Derive an explicit expression:

Original problem: $\mathbf{max}_{\alpha \in [0,C]^n} \quad -\frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y^i y^j\, k(x^i, x^j) + \sum_i \alpha_i$

# SVM Optimization in the Dual

What's the complexity of the update step? Derive an explicit expression:

Original problem: $\mathbf{max}_{\alpha\in[0,C]^n} \quad -\frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y^i y^j\, k(x^i,x^j)+\sum_i \alpha_i$

When all $\alpha_j$ except $\alpha_i$ are fixed: $\mathbf{max}_{\alpha_i\in[0,C]}\, F(\alpha_i)$, with

$$F(\alpha_i) = -\frac{1}{2}\alpha_i^2 k(x^i,x^i) + \alpha_i\Big(1 - y^i\sum_{j\neq i}\alpha_j y^j\, k(x^i,x^j)\Big) + \text{const.}$$

$$\frac{\partial}{\partial\alpha_i}F(\alpha_i) = -\alpha_i k(x^i,x^i) + \Big(1 - y^i\sum_{j\neq i}\alpha_j y^j\, k(x^i,x^j)\Big) + \text{const.}$$

$$\alpha_i^{\text{opt}} = \alpha_i + \frac{1 - y^i\sum_{j=1}^n \alpha_j y^j\, k(x^i,x^j)}{k(x^i,x^i)}, \qquad \alpha_i = \begin{cases} 0 & \text{if } \alpha_i^{\text{opt}} < 0, \\ C & \text{if } \alpha_i^{\text{opt}} > C, \\ \alpha_i^{\text{opt}} & \text{otherwise.} \end{cases}$$

(except if $k(x^i,x^i)=0$, but then $k(x^i,x^j)=0$, so $\alpha_i$ has no influence)

Observation: each update has complexity $O(n)$.

# (Generalized) Linear SVM Optimization in the Dual

Let $k(x, \bar{x}) = \langle \phi(x), \phi(\bar{x}) \rangle_{\mathbb{R}^d}$ for explicitly known $\phi : \mathcal{X} \to \mathbb{R}^d$.

$$\alpha_i^{\text{opt}} = \alpha_i + \frac{1 - y^i \sum_j \alpha_j y^j \, k(x^i, x^j)}{k(x^i, x^i)},$$

remember $w = \sum_j \alpha_j y_j \phi(x^j)$

$$= \alpha_i + \frac{1 - y^i \langle w, \phi(x^i) \rangle}{\|\phi(x^i)\|^2},$$

- each update takes $O(d)$, independent of $n$
  - $\langle w, \phi(x^i) \rangle$ takes at most $O(d)$ for explicit $w \in \mathbb{R}^d, \phi(x^i) \in \mathbb{R}^d$
  - we must also take care that $w$ remains up to date (also at most $O(d)$)

# (Generalized) Linear SVM Optimization in the Dual

**SCDA for (Generalized) Linear SVMs [Hsieh, 2008]**

initialize $\alpha \leftarrow \mathbf{0}$, $w \leftarrow \mathbf{0}$

**for** $t = 1, \ldots, T$ **do**

$i \leftarrow$ random index (uniformly random or in epochs)

$$\delta \leftarrow \frac{1 - y^i \langle w, \phi(x^i) \rangle}{\|\phi(x^i)\|^2}$$

$$\alpha_i \leftarrow \begin{cases} 0, & \text{if } \alpha_i + \delta < 0, \\ C, & \text{if } \alpha_i + \delta > C, \\ \alpha_i + \delta, & \text{otherwise.} \end{cases}$$

$$w \leftarrow w + \delta y^i \phi(x^i)$$

**end for**

return $\alpha$, $w$

Properties:

- converges monotonically to global optimum
- complexity of each step is independent of $n$
- resembles stochastic gradient method, but **automatic step size**

You've trained a new predictor, $g : \mathcal{X} \to \mathcal{Y}$, and you want to tell the world how good it is. How to measure this?

**Reminder:**

- The average loss on the training set, $\frac{1}{|\mathcal{D}_{trn}|} \sum_{(x,y)\in\mathcal{D}_{trn}} \ell(y, g(x))$ tells us (almost) nothing about the future loss.
  Reporting it would be misleading as best.
- The relevant quantity is the expected risk,

$$\mathcal{R}(g) = \mathbb{E}_{(x,y)\sim p(x,y)}\ \ell(y, g(x))$$

  which unfornately we cannot compute, since $p(x, y)$ is unknown.
- If we have data $\mathcal{D}_{tst} \overset{i.i.d.}{\sim} p(x, y)$, we have,

$$\frac{1}{|\mathcal{D}_{tst}|} \sum_{(x,y)\in\mathcal{D}_{tst}} \ell(y, g(x)) \quad \overset{|\mathcal{D}_{tst}|\to\infty}{\longrightarrow} \quad \mathbb{E}_{(x,y)\sim p(x,y)}\ \ell(y, g(x))$$

- Problem: samples $\ell(y, g(x))$ must me independent, otherwise law of large numbers doesn't hold.
- Make sure that $g$ is independent of $\mathcal{D}_{tst}$.

## Classifier Training (idealized)

**input** training data $\mathcal{D}_{trn}$
**input** learning procedure $A$
$g \leftarrow A[\mathcal{D}]$ (apply $A$ with $\mathcal{D}$ as training set)
**output** resulting classifier $g : \mathcal{X} \rightarrow \mathcal{Y}$

## Classifier Evaluation

**input** trained classifier $g : \mathcal{X} \rightarrow \mathcal{Y}$
**input** test data $\mathcal{D}_{tst}$
apply $g$ to $\mathcal{D}_{tst}$ and measure performance $R_{tst}$
**output** performance estimate $R_{tst}$

## Classifier Training (idealized)

**input** training data $\mathcal{D}_{trn}$
**input** learning procedure $A$
$g \leftarrow A[\mathcal{D}]$ (apply $A$ with $\mathcal{D}$ as training set)
**output** resulting classifier $g : \mathcal{X} \to \mathcal{Y}$

## Classifier Evaluation

**input** trained classifier $g : \mathcal{X} \to \mathcal{Y}$
**input** test data $\mathcal{D}_{tst}$
apply $g$ to $\mathcal{D}_{tst}$ and measure performance $R_{tst}$
**output** performance estimate $R_{tst}$

**Remark:** In commercial applications, this is realistic:

- given some training set one builds a single system,
- one deploys it to the customers,
- the customers use it on their own data, and complain if disappointed

In research, one typically has no customer, but only a fixed amount of data to work with, so one *simulates* the above protocol.

## Classifier Training and Evaluation

**input** data $\mathcal{D}$
**input** learning method $A$
  split $\mathcal{D} = \mathcal{D}_{trn} \dot{\cup} \mathcal{D}_{tst}$ disjointly
  set aside $\mathcal{D}_{tst}$ to a safe place  // do not look at it
  $g \leftarrow A[\mathcal{D}_{trn}]$  // learn a predictor from $\mathcal{D}_{trn}$
  apply $g$ to $\mathcal{D}_{tst}$ and measure performance $R_{tst}$
**output** performance estimate $R_{tst}$

## Classifier Training and Evaluation

**input** data $\mathcal{D}$
**input** learning method $A$
  split $\mathcal{D} = \mathcal{D}_{trn} \dot{\cup} \mathcal{D}_{tst}$ disjointly
  set aside $\mathcal{D}_{tst}$ to a safe place  // do not look at it
  $g \leftarrow A[\mathcal{D}_{trn}]$  // learn a predictor from $\mathcal{D}_{trn}$
  apply $g$ to $\mathcal{D}_{tst}$ and measure performance $R_{tst}$
**output** performance estimate $R_{tst}$

**Remark.** $\mathcal{D}_{tst}$ should be as small as possible, to keep $\mathcal{D}_{trn}$ as big as possible, but large enough to be convincing.

- sometimes: 50%/50% for small datasets
- more often: 80% training data, 20% test data
- for large datasets: 90% training, 10% test data.

**Remark:** The split because $\mathcal{D}_{trn}$ and $\mathcal{D}_{tst}$ must be absolute.

- Do not use $\mathcal{D}_{tst}$ for anything except the very last step.
- Do not look at $\mathcal{D}_{tst}$! Even if the learning algorithm doesn't see it, you looking at it can and will influence your model design or parameter selection (human overfitting).
- In particular, this applies to datasets that come with predefined set of test data, such as MNIST, PASCAL VOC, ImageNet, etc.

**Remark:** The split because $\mathcal{D}_{trn}$ and $\mathcal{D}_{tst}$ must be absolute.

- Do not use $\mathcal{D}_{tst}$ for anything except the very last step.
- Do not look at $\mathcal{D}_{tst}$! Even if the learning algorithm doesn't see it, you looking at it can and will influence your model design or parameter selection (human overfitting).
- In particular, this applies to datasets that come with predefined set of test data, such as MNIST, PASCAL VOC, ImageNet, etc.

In practice we often want more: not just evaluate one classifier, but

- select the best algorithm or parameters amongst multiple ones

We simulate the classifier evaluation step during the training procedure. This needs (at least) one additional data split:

## Training and Selecting between Multiple Models

**input** data $\mathcal{D}$
**input** set of method $\mathcal{A} = \{A_1, \ldots, A_K\}$
  split $\mathcal{D} = \mathcal{D}_{trnval} \dot{\cup} \mathcal{D}_{tst}$ disjointly
  set aside $\mathcal{D}_{tst}$ to a safe place (do not look at it)

  split $\mathcal{D}_{trnval} = \mathcal{D}_{trn} \dot{\cup} \mathcal{D}_{val}$ disjointly
  **for all** models $A_i \in \mathcal{A}$ **do**
    $g_i \leftarrow A_i[\mathcal{D}_{trn}]$
    apply $g_i$ to $\mathcal{D}_{val}$ and measure performance $E_{val}(A_i)$
  **end for**
  pick best performing $A_i$

  (optional) $g_i \leftarrow A_i[\mathcal{D}_{trnval}]$  // retrain on larger dataset
  apply $g_i$ to $\mathcal{D}_{tst}$ and measure performance $R_{tst}$
**output** performance estimate $R_{tst}$

How to split? For example $1/3$–$1/3$–$1/3$ or 70%–10%–20%.

**Discussion.**

- Each algorithm is trained on $\mathcal{D}_{trn}$ and evaluated on disjoint $\mathcal{D}_{val}$ ✓
- You select a predictor based on $E_{val}$ (its performance on $\mathcal{D}_{val}$), only afterwards $\mathcal{D}_{tst}$ is used. ✓
- $\mathcal{D}_{tst}$ is used to evaluate the final predictor and nothing else. ✓

**Discussion.**

- Each algorithm is trained on $\mathcal{D}_{trn}$ and evaluated on disjoint $\mathcal{D}_{val}$ ✓
- You select a predictor based on $E_{val}$ (its performance on $\mathcal{D}_{val}$), only afterwards $\mathcal{D}_{tst}$ is used. ✓
- $\mathcal{D}_{tst}$ is used to evaluate the final predictor and nothing else. ✓

**Problems.**

- small $\mathcal{D}_{val}$ is bad: $E_{val}$ could be bad estimate of $g_A$'s true performance, and we might pick a suboptimal method.
- large $\mathcal{D}_{val}$ is bad: $\mathcal{D}_{trn}$ is much smaller than $\mathcal{D}_{trnval}$, so the classifier learned on $\mathcal{D}_{trn}$ might be much worse than necessary.
- retraining the best model on $\mathcal{D}_{trnval}$ might overcome that, but it comes at a risk: just because a model worked well when trained on $\mathcal{D}_{trn}$, this does not mean it'll also work well when trained on $\mathcal{D}_{trnval}$.

## Leave-one-out Evaluation (for a single model/algorithm)

**input** algorithm $A$
**input** loss function $\ell$
**input** data $\mathcal{D}$ (trnval part only: test part set aside earlier)
  **for all** $(x^i, y^i) \in \mathcal{D}$ **do**
    $g^{\neg i} \leftarrow A[\ \mathcal{D} \setminus \{(x^i, y^i)\}\ ]$ // $\mathcal{D}_{trn}$ is $\mathcal{D}$ with $i$-th example removed
    $r^i \leftarrow \ell(y^i, g^{\neg i}(x^i))$ // $\mathcal{D}_{val} = \{(x^i, y^i)\}$, disjoint to $\mathcal{D}_{trn}$
  **end for**
**output** $R_{loo} = \frac{1}{n} \sum_{i=1}^{n} r^i$ (average leave-one-out risk)

**Properties.**

- Each $r^i$ is a unbiased (but noisy) estimate of the risk $\mathcal{R}(g^{\neg i})$
- $\mathcal{D} \setminus \{(x^i, y^i)\}$ is almost the same as $\mathcal{D}$, so we can hope that each $g^{\neg i}$ is almost the same as $g = A[\mathcal{D}]$.
- Therefore, $R_{loo}$ can be expected a good estimate of $\mathcal{R}(g)$

**Problem:** slow, trains $n$ times on $n-1$ examples instead of once on $n$

Compromise: use fixed number of small $\mathcal{D}_{val}$

## $K$-fold Cross Validation (CV)

**input** algorithm $A$, loss function $\ell$, data $\mathcal{D}$ (trnval part)
  split $\mathcal{D} = \dot{\bigcup}_{k=1}^{K} \mathcal{D}_k$ into $K$ equal sized disjoint parts
  **for** $k = 1, \ldots, K$ **do**
    $g^{\neg k} \leftarrow A[\,\mathcal{D} \setminus \mathcal{D}_k\,]$
    $r^k \leftarrow \frac{1}{|\mathcal{D}_k|} \sum_{(x,y)\in\mathcal{D}_k} \ell(y^i, g^{\neg k}(x))$
  **end for**
**output** $R_{K\text{-CV}} = \frac{1}{K} \sum_{k=1}^{n} r^k$ ($K$-fold cross-validation risk)

**Observation.**

- for $K = |\mathcal{D}|$ same as leave-one-out error.
- approximately $k$ times increase in runtime.
- most common: $k = 10$ or $k = 5$.

**Problem**: training sets overlap, so the error estimates are correlated.
Exception: $K = 2$

## $5 \times 2$ Cross Validation ($5 \times 2$-CV)

**input** algorithm $A$, loss function $\ell$, data $\mathcal{D}$ (trnval part)
  **for** $k = 1, \ldots, 5$ **do**
    Split $\mathcal{D} = \mathcal{D}_1 \dot{\cup} \mathcal{D}_2$
    $g_1 \leftarrow A[\mathcal{D}_1]$,
    $r_1^k \leftarrow$ evaluate $g_1$ on $\mathcal{D}_2$
    $g_2 \leftarrow A[\mathcal{D}_2]$,
    $r_2^k \leftarrow$ evaluate $g_2$ on $\mathcal{D}_1$
    $r^k \leftarrow \frac{1}{2}(r_k^1 + r_k^2)$
  **end for**
**output** $E_{5\times 2} = \frac{1}{5} \sum_{k=1}^{5} r^k$

**Observation.**

- $5 \times 2$-CV is really the average of $5$ runs of $2$-fold CV
- very easy to implement: shuffle the data and split into halfs
- within each run the training sets are disjoint and the classifiers $g_1$ and $g_2$ are independent

**Problem:** training sets are smaller than in $5$- or $10$-fold CV.

## Acknowledgement

Some slides are in courtesy of
the slides of C19 Machine Learning lectures by Prof. Andrew Zisserman (Oxford University)