

# Statistical Machine Learning

Christoph Lampert



*Institute of Science and Technology*

Spring Semester 2013/2014 // Lecture 4

## Constructing Kernels

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

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

Easier: construct functions that are guaranteed to be kernels:

Construct explicitly:

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

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.

# Optimizing the SVM Dual (kernelized)

How to solve the QP

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

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

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  $i = 1 \dots, n$  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

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:

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

New augmented:

- linear:  $f(x) = \langle \tilde{w}, \tilde{x} \rangle_{\mathbb{R}^{d+1}}$ , 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  $i = 1, \dots, n$ ,

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

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  $i = 1, \dots, n$ ,

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

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,  $0 \leq \alpha_i \leq C$ , for  $i = 1, \dots, n$ .

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



## Stochastic Coordinate Dual Ascent

```
 $\alpha \leftarrow \mathbf{0}.$   
for  $t = 1, \dots, T$  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:  $\max_{\alpha \in [0, C]^n} -\frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y^i y^j k(x^i, x^j) + \sum_i \alpha_i$

## SVM Optimization in the Dual

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

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

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

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

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

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

(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  $\phi : \mathcal{X} \rightarrow \mathbb{R}^d$ .

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

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**  $t = 1, \dots, T$  **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**

Practical Interlude:  
Doing Machine Learning Experiments

You've trained a new predictor,  $g : \mathcal{X} \rightarrow \mathcal{Y}$ , 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,

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

which unfortunately we cannot compute, since  $p(x, y)$  is unknown.

- If we have data  $\mathcal{D}_{tst} \stackrel{i.i.d.}{\sim} p(x, y)$ , we have,

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

- Problem: function  $c$  must be independent of  $\mathcal{D}_{tst}$ , otherwise law of large numbers doesn't hold.

## 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  $g : \mathcal{X} \rightarrow \mathcal{Y}$

## 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  $R_{tst}$

**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  $\mathcal{A} = \{A_1, \dots, A_K\}$

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  $\mathcal{D}$  (train/val part)  
split  $\mathcal{D} = \dot{\bigcup}_{k=1}^K \mathcal{D}_k$  into  $K$  equal sized disjoint parts  
**for**  $k = 1, \dots, K$  **do**  
     $g^{-k} \leftarrow A[\mathcal{D} \setminus \mathcal{D}_k]$   
     $r^k \leftarrow \frac{1}{|\mathcal{D}_k|} \sum_{(x,y) \in \mathcal{D}_k} \ell(y^i, g^{-k}(x))$   
**end for**  
**output**  $R_{K-CV} = \frac{1}{K} \sum_{k=1}^n r^k$  ( $K$ -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**  $k = 1, \dots, 5$  **do**

Split  $\mathcal{D} = \mathcal{D}_1 \dot{\cup} \mathcal{D}_2$

$g_1 \leftarrow A[\mathcal{D}_1]$ ,

$r_1^k \leftarrow \text{evaluate } g_1 \text{ on } \mathcal{D}_2$

$g_2 \leftarrow A[\mathcal{D}_2]$ ,

$r_2^k \leftarrow \text{evaluate } g_2 \text{ on } \mathcal{D}_1$

$r^k \leftarrow \frac{1}{2}(r_1^k + r_2^k)$

**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 halves
- 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.

# Classifiers for Information Retrieval Tasks

Some classification tasks are really rather *retrieval* tasks, e.g.

- database lookup: is an entry  $x$  relevant ( $y = 1$ ) or not ( $y = -1$ )?

A typical property:

- prediction is performed on a fixed database
- we have access to all elements of the prediction set at the same time
- positives ( $y = 1$ ) are important, negative ( $y = -1$ ) are a nuisance
- we don't need all decisions, a few correct positives is enough

For a classifier  $g(x) = \text{sign } f(x)$  with  $f(x) : \mathcal{X} \rightarrow \mathbb{R}$  (e.g.,  $f(x) = \langle w, x \rangle$ ), we interpret  $f(x)$  as its *confidence*.

To produce  $K$  positive we return the test samples of highest confidence.

Equivalently, we decide by  $g_\theta(x) = \text{sign}(f(x) - \theta)$ , for the right  $\theta$ .

## Other Ways to Evaluate Classifiers

Retrieval quality is often measure in terms of *precision* and *recall*:

### Definition (Precision, Recall, F-Score)

For  $\mathcal{Y} = \{\pm 1\}$ , let  $g : \mathcal{X} \rightarrow \mathcal{Y}$  a decision function and  $\mathcal{D} = \{(x^1, y^1), \dots, (x^n, y^n)\} \subset \mathcal{X} \times \mathcal{Y}$  be a *database*.

Then we define

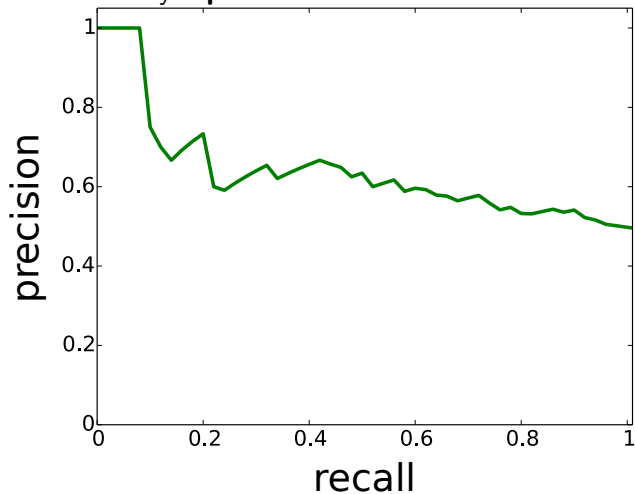
$$\text{precision}(g) = \frac{\text{number of test samples with } g(x^j) = 1 \text{ and } y^j = 1}{\text{number of test samples with } g(x^j) = 1}$$

$$\text{recall}(g) = \frac{\text{number of test samples with } g(x^j) = 1 \text{ and } y^j = 1}{\text{number of test samples with } y^j = 1}$$

$$F\text{-score}(g) = 2 \frac{\text{precision}(g) \cdot \text{recall}(g)}{\text{precision}(g) + \text{recall}(g)}$$

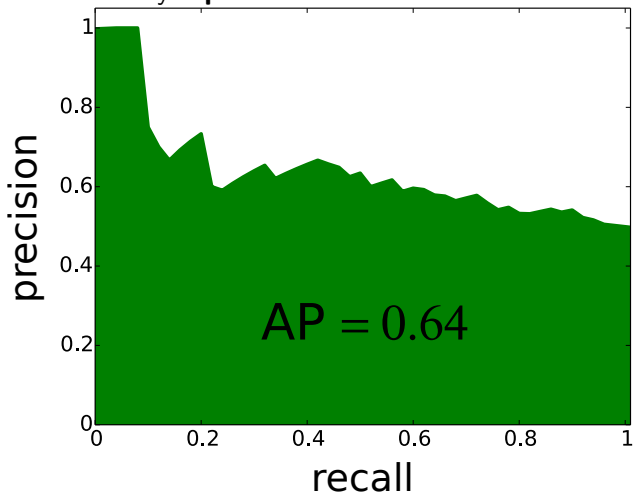
For different thresholds,  $\theta$ , we obtain different precision and recall values.

They are summarized by a **precision-recall curve**:



For different thresholds,  $\theta$ , we obtain different precision and recall values.

They are summarized by a **precision-recall curve**:



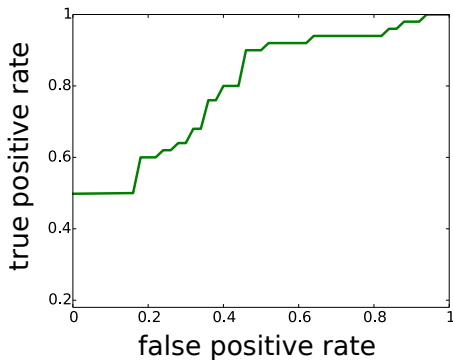
If pressured, summarize into one number: **average precision**.

A similar role in different context:

## Receiver Operating Characteristic (ROC) Curve

$$\text{true-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = 1}{\text{number of samples with } y^j = 1}$$

$$\text{false-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = -1}{\text{number of samples with } y^j = -1}$$



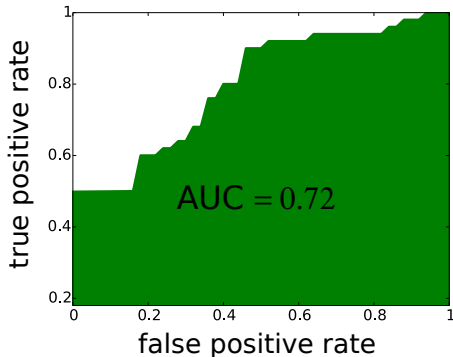


A similar role in different context:

## Receiver Operating Characteristic (ROC) Curve

$$\text{true-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = 1}{\text{number of samples with } y^j = 1}$$

$$\text{false-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = -1}{\text{number of samples with } y^j = -1}$$



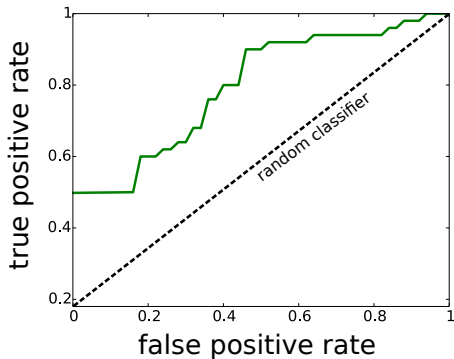
Summarize into: **area under ROC curve (AUC).**

A similar role in different context:

## Receiver Operating Characteristic (ROC) Curve

$$\text{true-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = 1}{\text{number of samples with } y^j = 1}$$

$$\text{false-positive-rate}(g) = \frac{\text{number of samples with } g(x^j) = 1 \text{ and } y^j = -1}{\text{number of samples with } y^j = -1}$$



Random classifier:  $AUC = 0.5$ , regardless of class proportions.

Some useful inequalities for next week...

# Measure Concentration Inequalities

- $Z$  random variables, taking values  $z \in \mathcal{Z} \subseteq \mathbb{R}$ .
- $p(Z = z)$  probability distribution
  - ▶  $\mu = \mathbb{E}[Z]$  mean
  - ▶  $\text{Var}[z] = \mathbb{E}[(Z - \mu)^2]$  variance

## Lemma

Let  $Z_1, \dots$ , be i.i.d. random variables with mean  $\mu$ , then

$$\frac{1}{m} \sum_{i=1}^m Z_i \xrightarrow[m \rightarrow \infty]{} \mu \quad \text{with probability 1.}$$

**Measure concentration inequalities** quantify the deviation between the two values for finite  $m$ .

# Markov's Inequality

Assumption:  $Z \subseteq \mathbb{R}_+$ , i.e.  $Z$  takes only non-negative values.

Observation 1) We can write

## Lemma (Markov's inequality)

$$\forall a \geq 0 : \quad \mathbb{P}[Z \geq a] \leq \frac{\mathbb{E}[Z]}{a}.$$

Example: Is it possible that more than half of the population have above-average salaries? No, by  $a = \frac{1}{2}\mu$ .

# Chebyshev's Inequality

## Lemma (Chebyshev's inequality)

$$\forall a \geq 0 : \quad \mathbb{P}[|Z - \mathbb{E}[Z]| \geq a] \leq \frac{\text{Var}[Z]}{a^2}$$

**Proof.** We apply Markov's Inequality to the random variable  $(Z - \mathbb{E}[Z])^2$ .

For any  $a \geq 0$ :

$$\mathbb{P}[|Z - \mathbb{E}[Z]| \geq a] = \mathbb{P}[(Z - \mathbb{E}[Z])^2 \geq a^2] \stackrel{\text{Markov}}{\leq} \frac{\mathbb{E}[(Z - \mathbb{E}[Z])^2]}{a^2} = \frac{\text{Var}[Z]}{a^2}.$$

# Applying Chebyshev's Inequality

## Lemma

Set  $Z_1, \dots, Z_m$  be i.i.d. random variables with  $\mathbb{E}[Z_i] = \mu$  and  $\text{Var}[Z_i] \leq 1$ . Then, for any  $\delta \in (0, 1)$  the following inequality holds with probability at least  $1 - \delta$ :

$$\left| \frac{1}{m} \sum_{i=1}^m Z_i - \mu \right| \leq \sqrt{\frac{1}{\delta m}}.$$

**Proof.** The  $Z_i$  are i.i.d., so  $\text{Var} \left[ \frac{1}{m} \sum_{i=1}^m Z_i \right] = \frac{1}{m} \sum_{i=1}^m \text{Var}[Z_i] \leq 1$ .

Chebyshev's inequality give us for any  $a > 0$

$$\mathbb{P} \left[ \left| \frac{1}{m} \sum_{i=1}^m Z_i - \mu \right| > a \right] \leq \frac{\text{Var} \left[ \frac{1}{m} \sum_{i=1}^m Z_i \right]}{ma^2} \leq \frac{1}{ma^2}.$$

Setting  $\delta = \frac{1}{ma^2}$  and solving for  $a$  yields  $a = \sqrt{\frac{1}{\delta m}}$ .

# Chernoffs' Bound

## Lemma (Multiplicative Chernoff Bound)

Let  $Z_1, \dots, Z_m$  be independent Bernoulli (i.e. 0/1-values) variables, with  $\mathbb{P}[Z_i = 1] = p_i$  and  $\mathbb{P}[Z_i = 0] = 1 - p_i$  for any  $i$ . Let  $p = \sum_{i=1}^m p_i$  and  $Z = \sum_{i=1}^m Z_i$ . Then, for any  $\delta > 0$ ,

$$\mathbb{P}[Z > (1 + \delta)p] \leq e^{-h(\delta)p}$$

and

$$\mathbb{P}[Z < (1 - \delta)p] \leq e^{-h(-\delta)p}$$

where  $h(\delta) = (1 + \delta) \log(1 + \delta) - \delta$ .

Using  $h(\delta) \geq \frac{\delta^2}{2+2\delta/3}$  one sees that

$$\mathbb{P}[Z > (1 + \delta)p] \leq e^{-p \frac{\delta^2}{2+2\delta/3}} \quad \text{and} \quad \mathbb{P}[Z < (1 - \delta)p] \leq e^{-p \frac{\delta^2}{2-2\delta/3}}$$

which shows that the probability drops *exponentially* in  $\delta$ .



# Hoeffding's Lemma and Inequality

## Lemma (Hoeffding's Lemma)

*Let  $Z$  be a random variable that takes values in  $[a, b]$  and  $\mathbb{E}[Z] = 0$ . Then, for every  $\lambda > 0$ ,*

$$\mathbb{E}[e^{\lambda Z}] \leq e^{\frac{\lambda^2(b-a)^2}{8}}.$$

## Lemma (Hoeffding's Inequality)

*Let  $Z_1, \dots, Z_m$  be i.i.d. random variables that take values in the interval  $[a, b]$ . Let  $\bar{Z} = \frac{1}{m} \sum_{i=1}^m Z_i$  and denote  $\mathbb{E}[\bar{Z}] = \mu$ . Then, for any  $\epsilon > 0$ ,*

$$\mathbb{P}\left[\left|\frac{1}{m} \sum_{i=1}^m Z_i - \mu\right| > \epsilon\right] \leq 2e^{-m \frac{\epsilon^2}{(b-a)^2}}.$$