SVMs, Kernelized SVMs

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Outline

1. Review of last lecture
2. SVM – Hinge loss
3. Kernelized SVMs
4. Evaluating ML algorithms

Support Vector Machine

- A linear classifier (hyperplane) that maximizes the margin.
- An alternative view of SVMs.

Outline

A general view of supervised learning

Definition Assume $y \in \{-1, 1\}$ and the decision rule is $h(\boldsymbol{x}) = \textsc{sign}(a(\boldsymbol{x}))$ with $a(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}) + b$

For classification: $0/1$ loss

$$\ell^{0/1}(y, a(\boldsymbol{x})) = \begin{cases} 0 & \text{if } ya(\boldsymbol{x}) \geq 0 \\ 1 & \text{otherwise} \end{cases}$$

Minimize weighted sum of empirical risk and regularizer

$$
\begin{aligned}
&\arg\min_{\boldsymbol{w},b} R^{\text{EMP}}[h_{\boldsymbol{w},b}(x)] + \lambda R(\boldsymbol{w}, b) \\
&= \arg\min_{\boldsymbol{w},b} \frac{1}{N} \sum_n \ell(y_n, a(\boldsymbol{x}_n)) + \lambda R(\boldsymbol{w}, b)
\end{aligned}
\tag{1}
$$

Minimize weighted sum of empirical risk and regularizer

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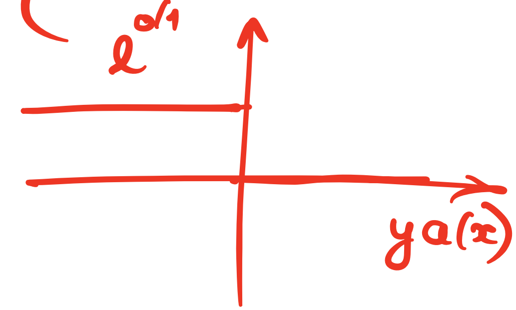

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\end{aligned}
$$

- Problem with minimizing the $0/1$ loss ?

Hinge loss

Definition Assume $y \in \{-1, 1\}$ and the decision rule is $h(\boldsymbol{x}) = \text{SIGN}(a(\boldsymbol{x}))$ with $a(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}) + b$,

$$\ell^{\text{HINGE}}(y, a(\boldsymbol{x})) = \begin{cases} 0 & \text{if } ya(\boldsymbol{x}) \geq 1 \\ 1 - ya(\boldsymbol{x}) & \text{otherwise} \end{cases}$$

Intuition

$ya(x) < 0$

$ya(x) \geq 0$

$ya(x) < 1$

Hinge loss

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Intuition

- No penalty if raw output, $a(\boldsymbol{x})$, has same sign and is far enough from decision boundary (i.e., if 'margin' is large enough)
- Otherwise pay a growing penalty, between 0 and 1 if signs match, and greater than one otherwise

Hinge loss

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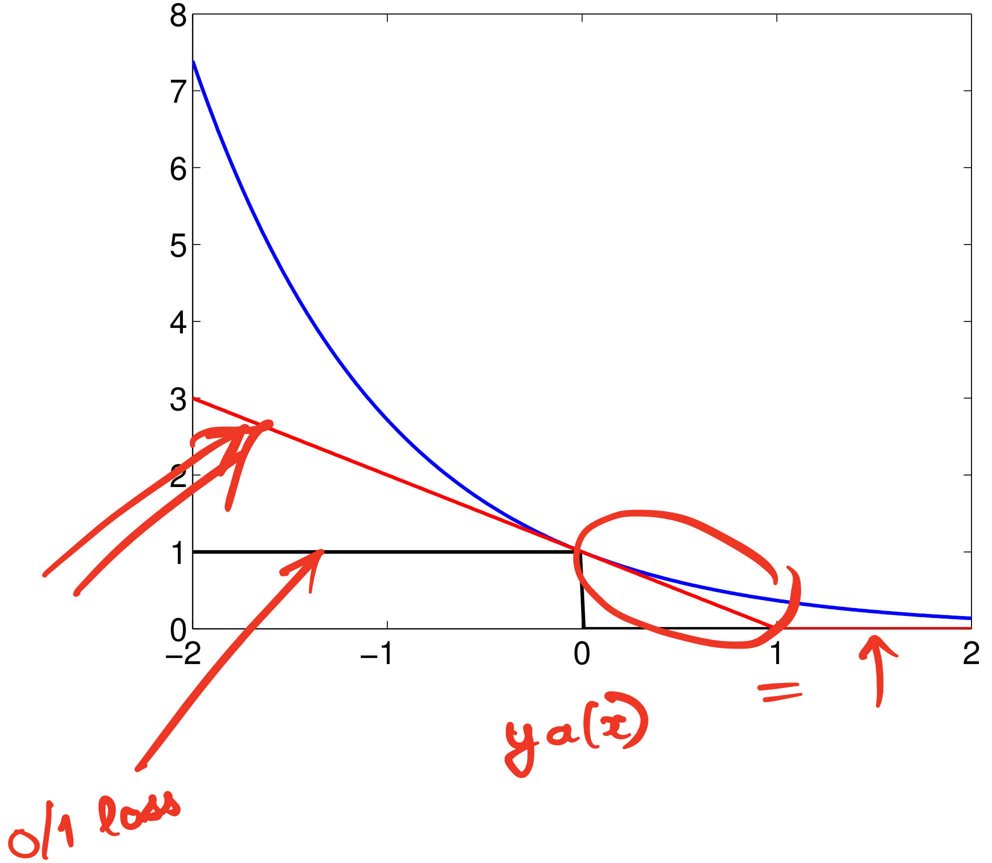
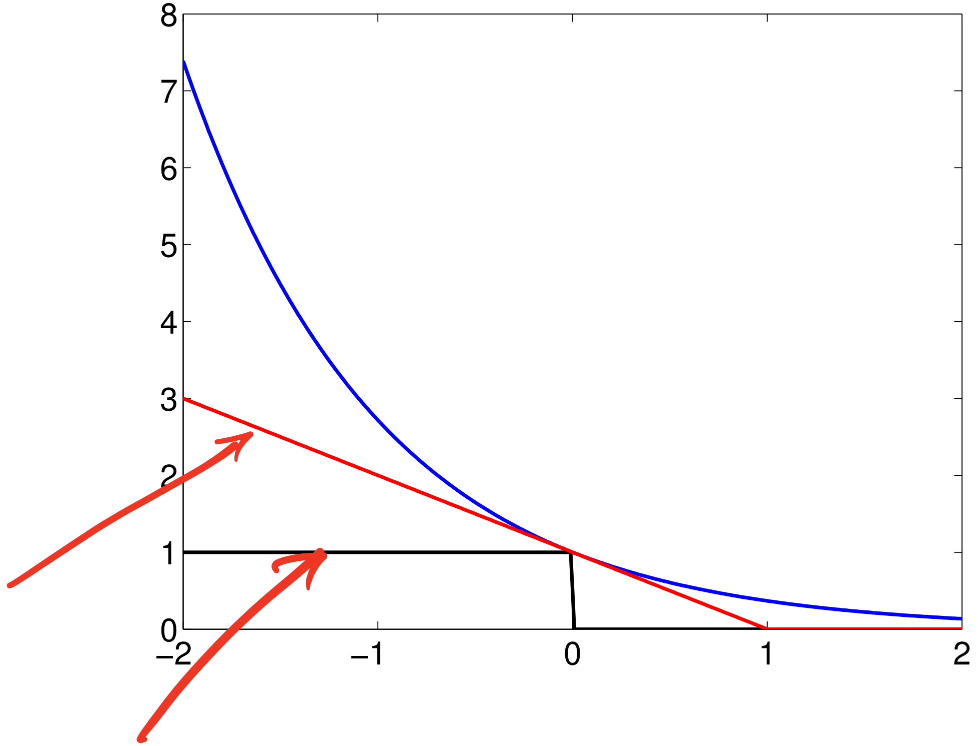
Convenient shorthand

$$\ell^{\text{HINGE}}(y, a(\boldsymbol{x})) = \max(0, 1 - ya(\boldsymbol{x})) = (1 - ya(\boldsymbol{x}))_+$$

Visualization and Properties



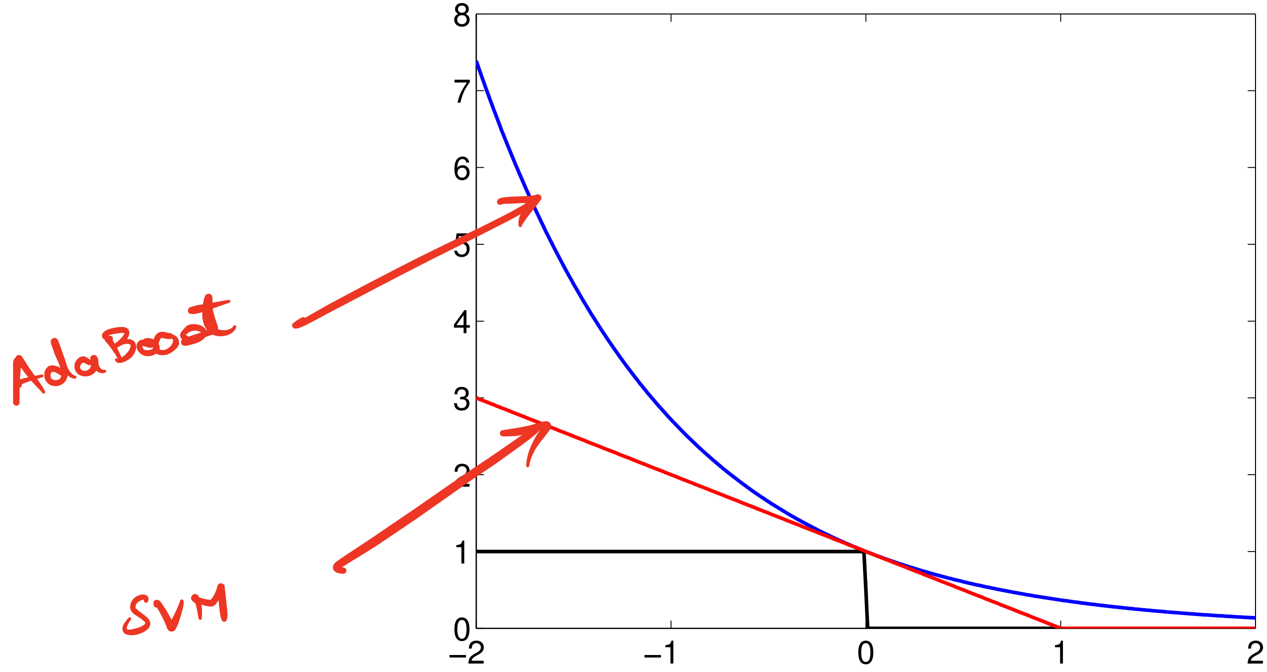
Visualization and Properties



- Upper-bound for $0/1$ loss function (black line)
- We use hinge loss as a *surrogate* to $0/1$ loss – Why?

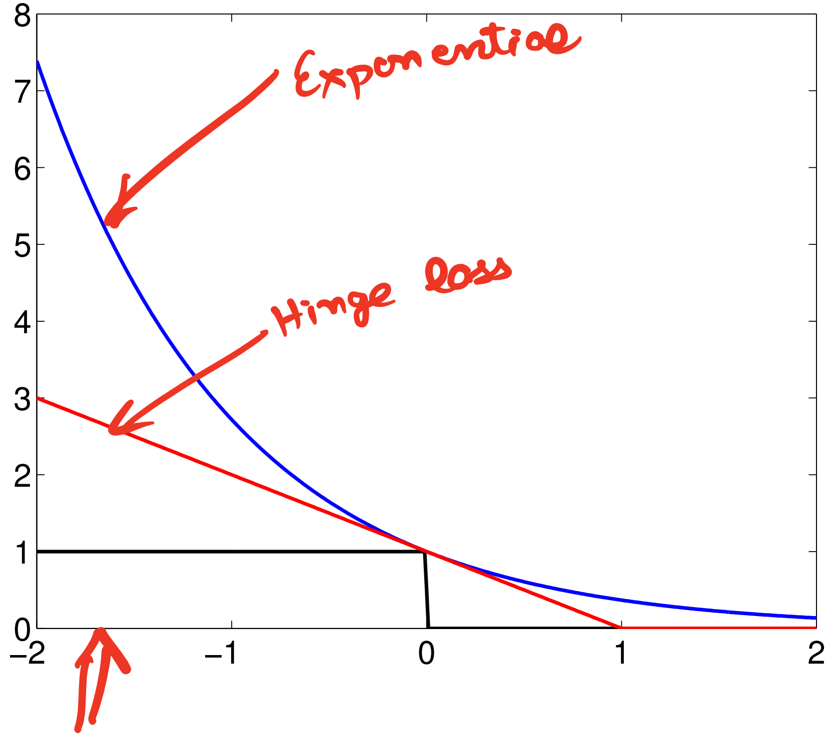
Visualization and Properties

Logistic loss → Logistic regression



- Upper-bound for $0/1$ loss function (black line)
- We use hinge loss as a *surrogate* to $0/1$ loss – Why?
- Hinge loss is convex, and thus easier to work with.

Visualization and Properties



- Other surrogate losses can be used, e.g., exponential loss for Adaboost (in blue), logistic loss (not shown) for logistic regression
- Hinge loss less sensitive to outliers than exponential (or logistic) loss

Primal formulation of support vector machines (SVM)

Minimizing the total hinge loss on all the training data with l_2 regularization

$$\min_{\boldsymbol{w},b} \sum_n \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]) + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

Analogous to l_2 regularized least squares, as we balance between two terms (the loss and the regularizer).

Hinge loss

(x_n, y_n)

$\max(0, 1 - y\,a(x))$

$a(x) = [w^T \phi(x) + b]$

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Analogous to l_2 regularized least squares, as we balance between two terms (the loss and the regularizer).

Previously, we used geometric arguments to derive:

Margin

Slack variables

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_n \xi_n$$

$$\text{s.t.} \quad y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0, \quad n \in \{1, \ldots, N\}$$

Do these yield the same solution?

Recovering our previous SVM formulation

Minimizing the total hinge loss on all the training data

$$\min_{\boldsymbol{w},b} \sum_n \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]) + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

Define $C = 1/\lambda$:

$$\min_{\boldsymbol{w},b} C\sum_n \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]) + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

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Define $\xi_n = \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b])$

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

$$\text{s.t.} \quad \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]) = \xi_n, \quad n \in \{1, \ldots, N\}$$

Recovering our previous SVM formulation

$(w^*, b^*), \{\xi_n^*\}$

Minimizing hinge loss

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

$$\text{s.t.} \quad \max(0, 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b]) = \xi_n, \quad n \in \{1, \ldots, N\}$$

is equivalent to

$\xi_n^* = \max(0, 1 - y_n(w^{*T}\phi(x_n) + b^*))$

SVM

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \left[C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 \right]$$

$$\text{s.t.} \quad 1 - y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] \leq \xi_n, \quad n \in \{1, \ldots, N\}$$

$$0 \leq \xi_n, \quad n \in \{1, \ldots, N\}$$

$\Rightarrow \xi_n \geq \max(0, 1 - y_n(w^T\phi(x_n) + b))$

$\Rightarrow \xi_n^* \geq \max(0, 1 - y_n(w^{*T}\phi(x_n) + b^*))$

At optimal solution constraints are active so we have equality! Why?

$$\xi_n^* \geq \max\left(0,\ 1 - y_n\left(w^{*T}\phi(x_n) + b^*\right)\right)$$

$$\tilde{\xi}_n$$

$$C \sum_n \xi_n + \frac{1}{2}\|w\|_2^2$$

At optimal solution constraints are active so we have equality! Why?

- If $\xi_n^* > \max(0, 1 - y_n f(\boldsymbol{x}_n))$, we could choose $\bar{\xi}_n < \xi_n^*$ and still satisfy the constraint while reducing our objective function!
- Since $c \geq \max(a, b) \iff c \geq a,\, c \geq b$, we recover previous formulation

SVM: hyperplane with largest margin

= minimizes Hinge loss

+ ℓ_2- regularization

Outline

Goal: Kernelize SVMs

$\phi(x_n)$

- Rewrite the SVM optimization problem so that it no longer depends on $\phi(\boldsymbol{x}_n)$ but instead depends only on inner products $\phi(\boldsymbol{x}_n)^{\mathrm{T}}\phi(\boldsymbol{x}_m)$.
- If we can do this, we can then replace $\phi(\boldsymbol{x}_n)^{\mathrm{T}}\phi(\boldsymbol{x}_m)$ with a kernel function $k(\boldsymbol{x}_n, \boldsymbol{x}_m)$.

Primal formulation of support vector machines (SVM)

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_n \xi_n$$

$$\text{s.t.} \quad y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] \geq 1 - \xi_n \quad \text{and} \quad \xi_n \geq 0, \quad n \in \{1, \ldots, N\}$$

This can be converted to its *dual form*.

Dual formulation of SVM

Let $\boldsymbol{w}_*$ be the minimizer of the SVM problem for training data: $\{(\boldsymbol{x}_n, y_n)\}$.

Then $\boldsymbol{w}_* = \sum_n \alpha_n y_n \phi(\boldsymbol{x}_n)$ for a new set of dual variables: $\alpha_n \geq 0$.

Primal

Dual

Dual formulation of SVM

$y_m \in \{+1, -1\}$

Dual is also a convex program

$\alpha = (\alpha_1, \ldots, \alpha_N)$

$$\max_{\boldsymbol{\alpha}} \left(\sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) \right)$$

$$\text{s.t.} \quad 0 \leq \alpha_n \leq C, \quad n \in 1, \ldots, N$$

$$\sum_n \alpha_n y_n = 0$$

There are N dual variable α_n, one for each constraint in the primal formulation

Kernel SVM

We replace the inner products $\phi(\boldsymbol{x}_m)^{\mathrm{T}}\phi(\boldsymbol{x}_n)$ with a kernel function

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \quad & \sum_n \alpha_n - \frac{1}{2}\sum_{m,n} y_m y_n \alpha_m \alpha_n k(\boldsymbol{x}_m, \boldsymbol{x}_n) \\ \text{s.t.} \quad & 0 \leq \alpha_n \leq C, \quad n \in 1, \ldots, N \\ & \sum_n \alpha_n y_n = 0 \end{aligned}$$

α_*

We can define a kernel function to work with nonlinear features and learn a nonlinear decision surface

Recovering solution to the primal formulation

$w^T \phi(x_n) + b$ $\quad$ $k(x, x_n)$

Weights w (primal variables) relation to α (dual variables)

$$w = \sum_n y_n \alpha_n \phi(x_n) \leftarrow$$ Linear combination of the input features

Prediction on a test point x

$$h(x) = \text{SIGN}(w^T \phi(x) + b) = \text{SIGN}(\sum_n y_n \alpha_n k(x_n, x) + b)$$

At test time it suffices to know the kernel function!

$$w = \sum_n y_n \alpha_n \phi(x_n)$$

$$w^T \phi(x) = \left(\sum_n y_n \alpha_n \phi(x_n)\right)^T \phi(x) = \sum_n y_n \alpha_n \phi(x_n)^T \phi(x)$$

Recovering solution to the primal formulation

We already identified the primal variable $\boldsymbol{w}$ as

$$\boldsymbol{w} = \sum_n \alpha_n y_n \boldsymbol{\phi}(\boldsymbol{x}_n)$$

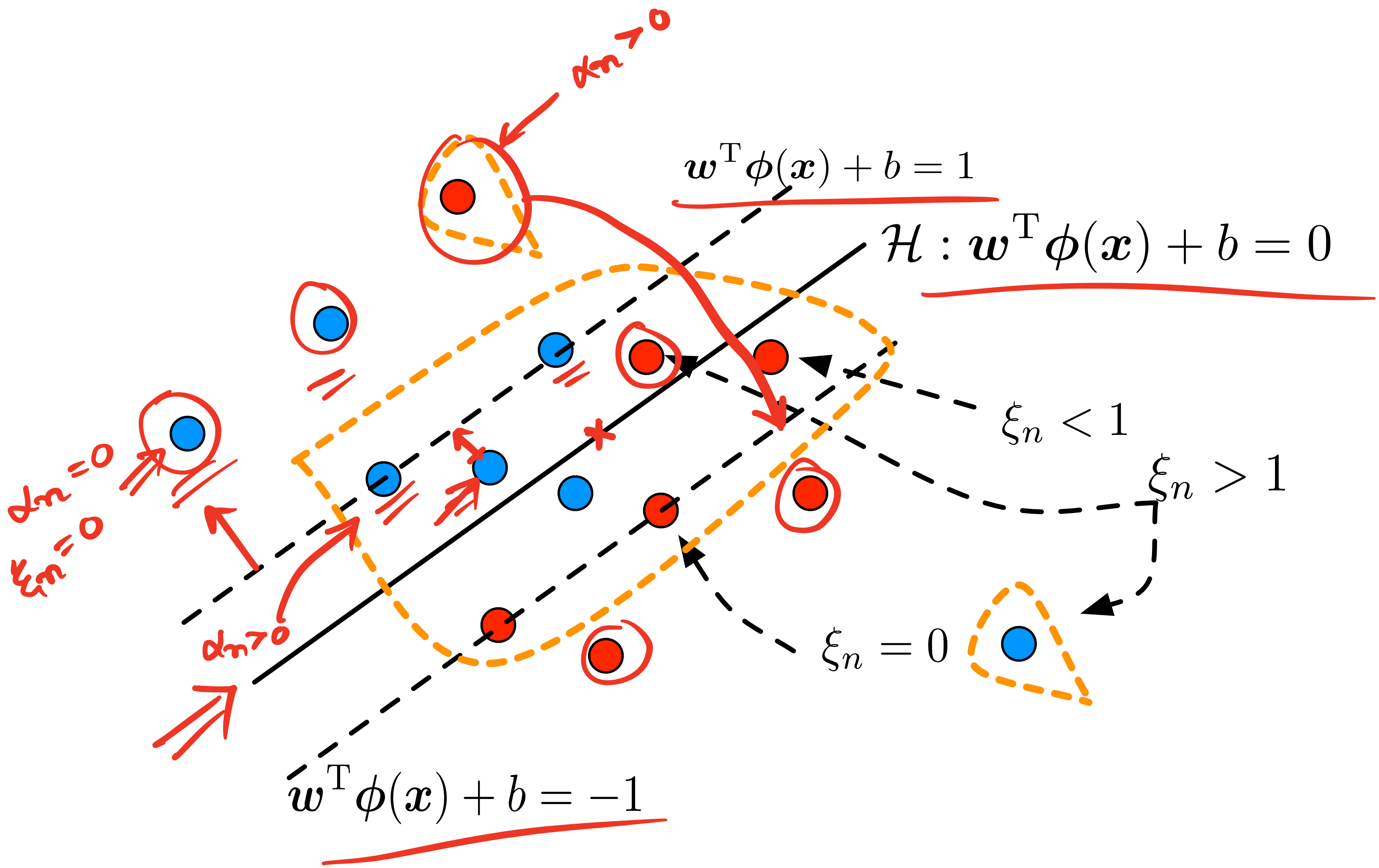
$0 \leq \alpha_n \leq C$

- From the dual, we know that $0 \leq \alpha_n \leq C$.
- If $\alpha_n = 0$, then the example n does not affect the hyperplane/decision boundary computed by SVM. $y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] \geq 1$.
- Only those examples with $\alpha_n > 0$ affect the hyerplane/decision boundary. These examples are termed support vectors.
- When will $\alpha_n > 0$?

$\xi_n \geq 0$

  - $\alpha_n = C \Rightarrow y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] \leq 1$.
  - $0 < \alpha_n < C \Rightarrow y_n[\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b] = 1$.

Visualization of how training data points are categorized



Support vectors are highlighted by the dotted orange lines

Outline

Binary classification

Goal is to achieve high accuracy

Accuracy: defined to be the mean of the $0/1$ loss $l(y, \hat{y})$.

$$\ell(y, h(\boldsymbol{x})) = \mathbf{1}\{y \neq h(\boldsymbol{x})\}$$

$$R^{\text{EMP}}[h(\boldsymbol{x})] = \frac{1}{N} \sum_{n} \ell(h(\boldsymbol{x}_n), y_n)$$

Assumes $y \in \{0, 1\}$ and h outputs values in $\{0, 1\}$.

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May not be what we want

Is this email spam?

Does the patient have cancer?

Confusion matrix

Given a dataset of P positive instances and N negative instances,

		Predicted class 1	Predicted class 0	
Actual class	1	TP	FN	P
	0	FP	TN	N

P = Positive, N = Negative
TN = True negative, FP = False positive
TP = True positive, FN = False negative

Spam classification

- Positive : spam, Negative: non-spam
- TP: Spam email classified as spam
- FP: Non-spam email classified as spam

Confusion matrix

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- Accuracy $= \frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{P}+\mathrm{N}}$
- Error = 1 - Accuracy

Confusion matrix

Given a dataset of P positive instances and N negative instances,

		Predicted class		
		1	0	
Actual	1	TP	FN	P
class	0	FP	TN	N

P = Positive, N = Negative
TN = True negative, FP = False positive
TP = True positive, FN = False negative

- True Positive Rate (TPR) = Recall = Sensitivity = $\frac{\mathrm{TP}}{\mathrm{P}}$
- Probability of classifying a spam email as spam.

Confusion matrix

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		1	0	
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class	0	FP	TN	N

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- Specificity $= \frac{\mathrm{TN}}{\mathrm{N}}$
- Probability of classifying a non-spam email as non-spam.
- False Positive Rate (FPR) = 1 - Specificity

Confusion matrix

Given a dataset of P positive instances and N negative instances,

		Predicted class		
		1	0	
Actual	1	TP	FN	P
class	0	FP	TN	N

P = Positive, N = Negative
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TP = True positive, FN = False negative

- Precision = Positive Predictive Value (PPV) = $\frac{\mathrm{TP}}{\mathrm{TP+FP}}$
- Probability that an email classified as spam is spam.
- Different from specificity!

Visualizing performance

Many different performance measures

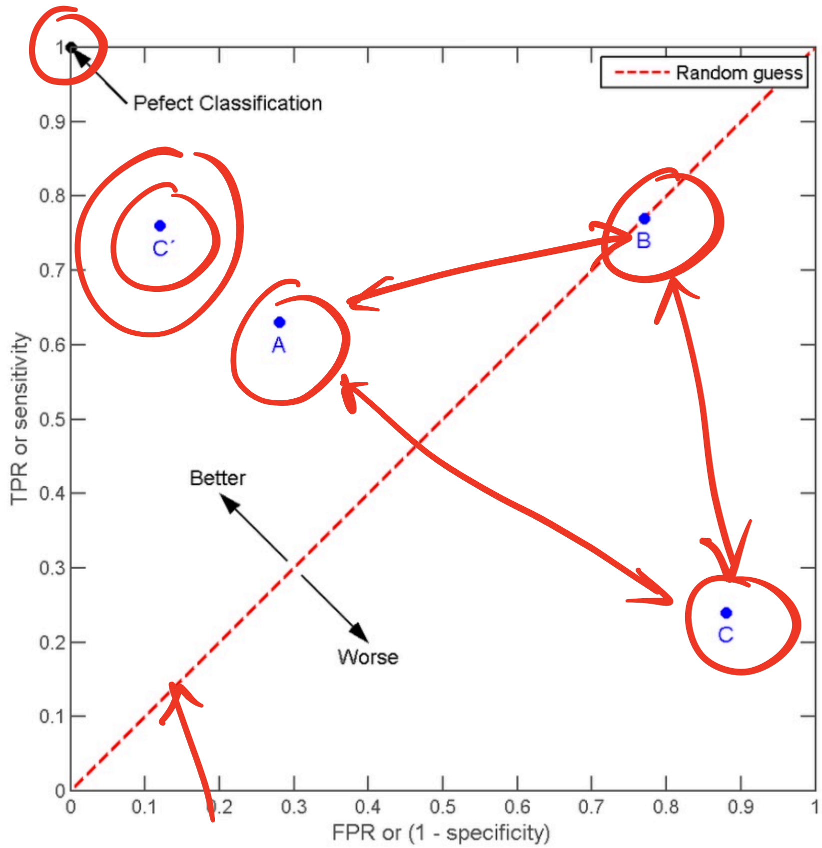
A			B			C			C′		
TP=63	FN=37	100	TP=77	FN=23	100	TP=24	FN=76	100	TP=76	FN=24	100
FP=28	TN=72	100	FP=77	TN=23	100	FP=88	TN=12	100	FP=12	TN=88	100
91	109	200	154	46	200	112	88	200	88	112	200

[1]

[1] https://en.wikipedia.org/wiki/Receiver_operating_characteristic

ROC curve

TPR (sensitivity) vs FPR (1-specificity)



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- Best possible method is in the upper left corner.
- Random guess would fall on the diagonal.

https://en.wikipedia.org/wiki/Receiver_operating_characteristic

Sometimes we care about the confidence of predictions

- For linear models (*e.g.*, perceptron, logistic regression), the activation $a(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b$ gives us a ranking of the predictions.
- In the case of the perceptron, given $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ such that $a(\boldsymbol{x}_1) > a(\boldsymbol{x}_2) > 0$.
  - Both $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ are classified as positive.
  - Perceptron is more confident in the prediction for $\boldsymbol{x}_1$ than for $\boldsymbol{x}_2$.

ROC curve allows us to visualize the ranking of predictions

Building a ROC curve

- Sort the instances according to the confidence of instance being in class 1 (positive class).
  - How confident is the classifier that an email is spam?

Building a ROC curve

- Sort the instances according to the confidence of instance being in class 1 (positive class).
  - How confident is the classifier that an email is spam?
- Step through the sorted list from high to low confidence.
- As you step through, build a binary classifier that predicts the top k instances as belonging to class 1 and the remaining to class 0.
  - How aggressively do you want to mark a message as spam ?

Building a ROC curve

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  - How aggressively do you want to mark a message as spam ?
- Compute the TPR (True Positive Rate) and FPR (False Positive Rate).
  - High up in the list: Low TPR and low FPR.
  - As we move down, TPR increases but so does FPR.

Building a ROC curve

- Sort the instances according to the confidence of instance being in class 1 (positive class).
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- Step through the sorted list from high to low confidence.
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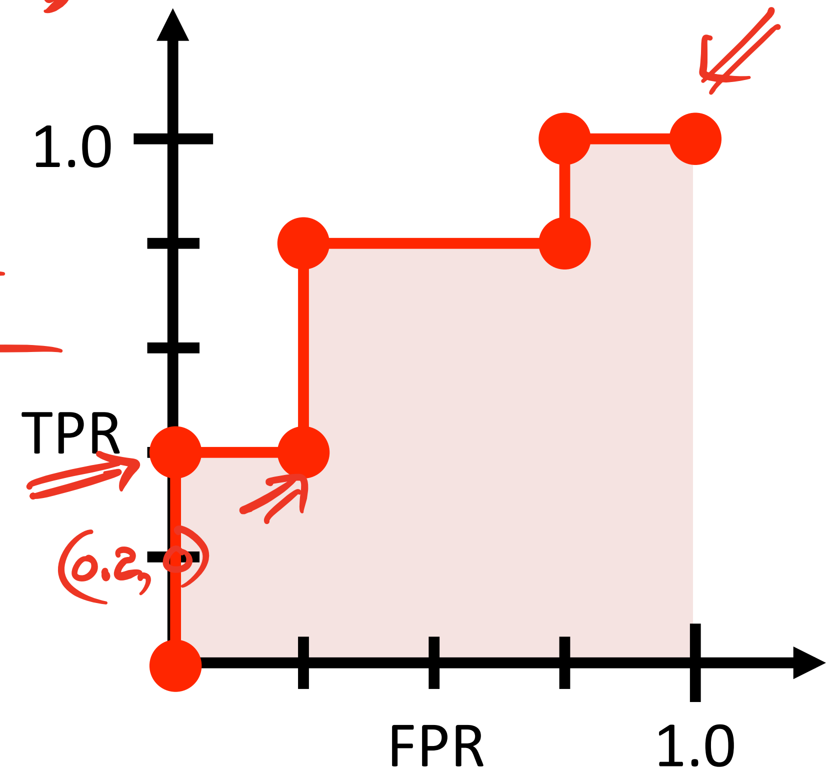
  - How aggressively do you want to mark a message as spam ?
- Compute the TPR (True Positive Rate) and FPR (False Positive Rate).
  - High up in the list: Low TPR and low FPR.
  - As we move down, TPR increases but so does FPR.
- Plot TPR vs FPR.

Example

$$TPR = \frac{TP}{\text{Positives}} = \frac{1}{5} \qquad FPR = 1 - \frac{TN}{\text{Negatives}} = 1 - \frac{5}{5} = 0$$

Instance	Confidence in positive	Actual class
9	0.99	1
7	0.98	1
1	0.72	0
2	0.70	1
6	0.65	1
10	0.51	0
3	0.39	0
5	0.24	1
4	0.11	0
8	0.01	0

$(\frac{2}{5}, 0)$

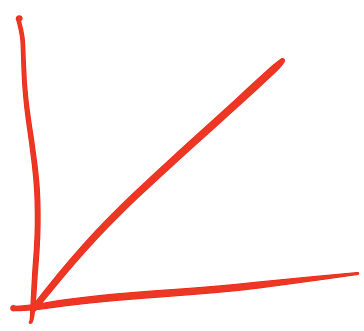


$$TPR = \frac{2}{5} \qquad FPR = \frac{1}{5}$$

Interpreting ROC curves

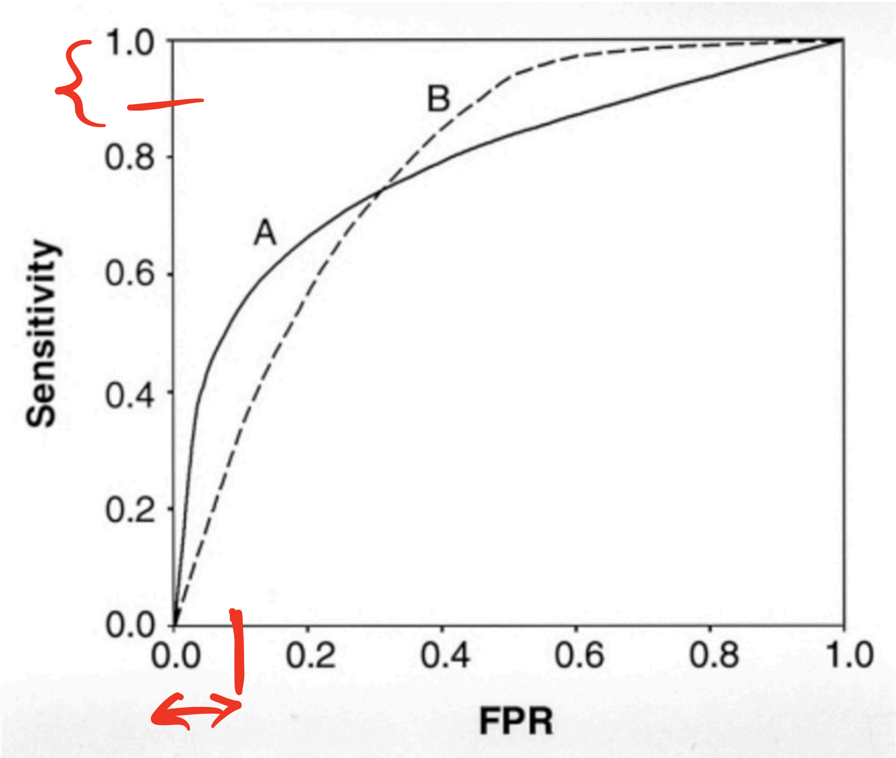
Area under the ROC Curve (AUC or AUROC)

- The probability that a classifier will rank a randomly chosen positive instance (instance with class label 1) higher than a randomly chosen negative one (instance with class label 0).
- A measure of the overall performance of a classifier.
- A random classifier has AUROC $= \frac{1}{2}$.
- A perfect classifier has AUROC $= 1$.



Interpreting ROC curves

Classifiers A and B with equal AUROC



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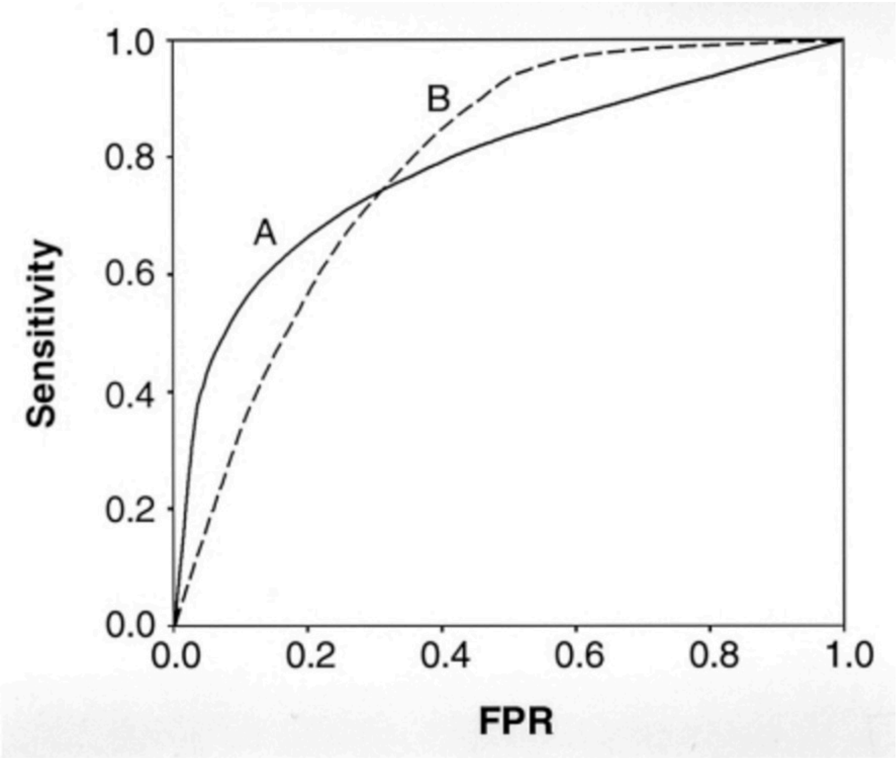
Which one do we choose?

Park et al. KJR 2004

Interpreting ROC curves

Classifiers A and B with equal AUROC



3

Which one do we choose?

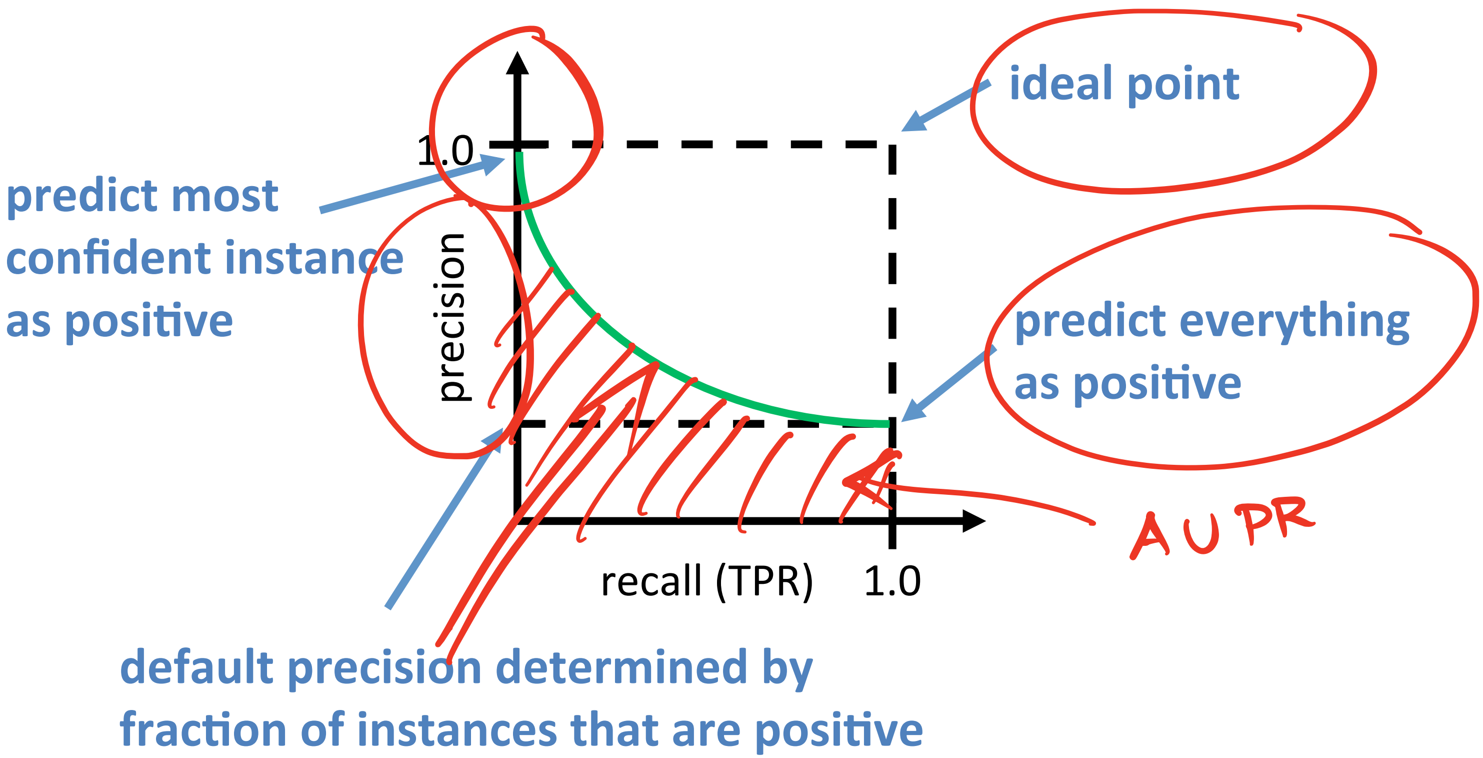
Depends on whether we care about sensitivity or FPR

Park et al. KJR 2004

Other trade-offs

$$\text{Precision} = \frac{TP}{TP + FP}$$

Precision-recall curve



Interpreting precision-recall curves

Area under the precision-recall curve (AUPR)

- Can compute the area under the precision-recall curve.

Interpreting precision-recall curves

F_1-score

$$F_1 = \frac{1}{\frac{1}{2}\frac{1}{\textsc{Precision}} + \frac{1}{2}\frac{1}{\textsc{Recall}}}$$

- Want F_1 to be high.
- The Harmonic mean of precision and recall.
- A single number that trades off precision and recall.
- If a classifier has high precision and low recall (or other way round), its F_1-score will be low.
- Encourages precision and recall values that are similar.

Summary

- Many ways to measure accuracy.
- Think carefully about which ones are most relevant.
- Often there are trade-offs
  - TPR vs FPR, Precision vs recall
- Graphical displays useful.
  - ROC and Precision-recall curves display performance at various levels of confidence.
  - Can be summarized by area under the curve (AUROC, AUPR) as well as numbers such as the F_1-score.