Beta calibration:

a well-founded and easily implemented improvement on logistic calibration for binary classifiers

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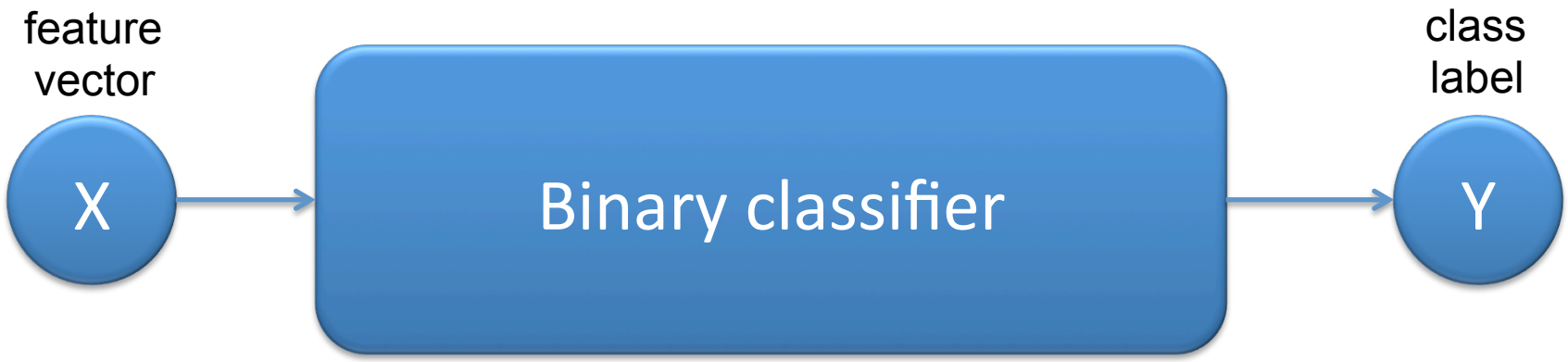
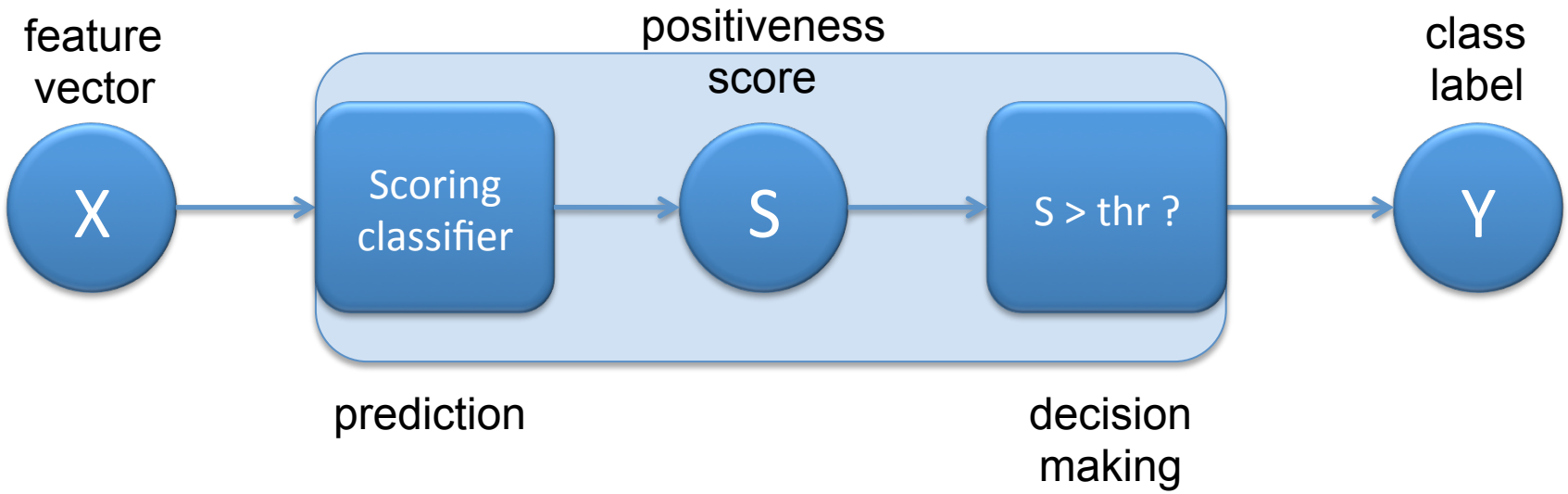
Prediction confidence of binary classifiers



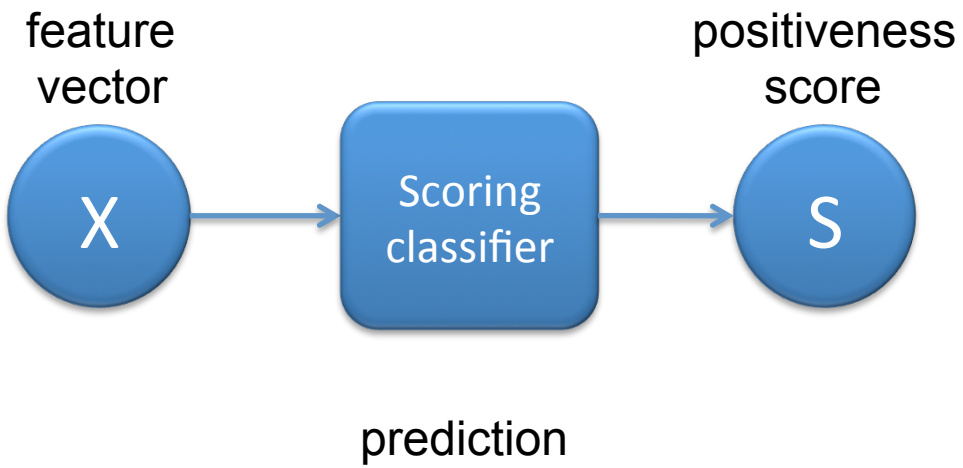
- Confidence use cases:
  - Abstaining classifier
  - Costs unknown during training
  - Human decision-maker
- Separation of prediction and decision-making

Score quantifies confidence in label



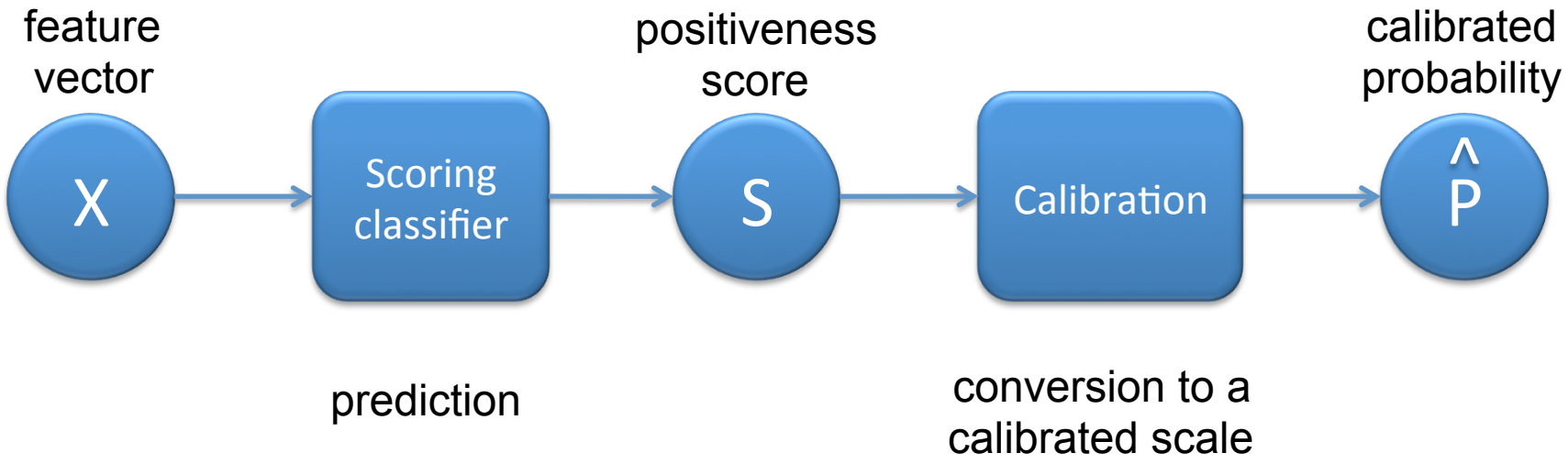
- Higher positiveness score S means more likely Y=1
  - SVM: signed distance to the decision boundary
  - Neural net: positive class probability from softmax
  - Naïve Bayes: positive class probability

Score quantifies confidence in label



- Higher positiveness score S means more likely Y=1
  - SVM: signed distance to the decision boundary
  - Neural net: positive class probability from softmax
  - Naïve Bayes: positive class probability
- Problem: the scale of S is model-dependent
  - How many positives among instances with S=0.8 ?

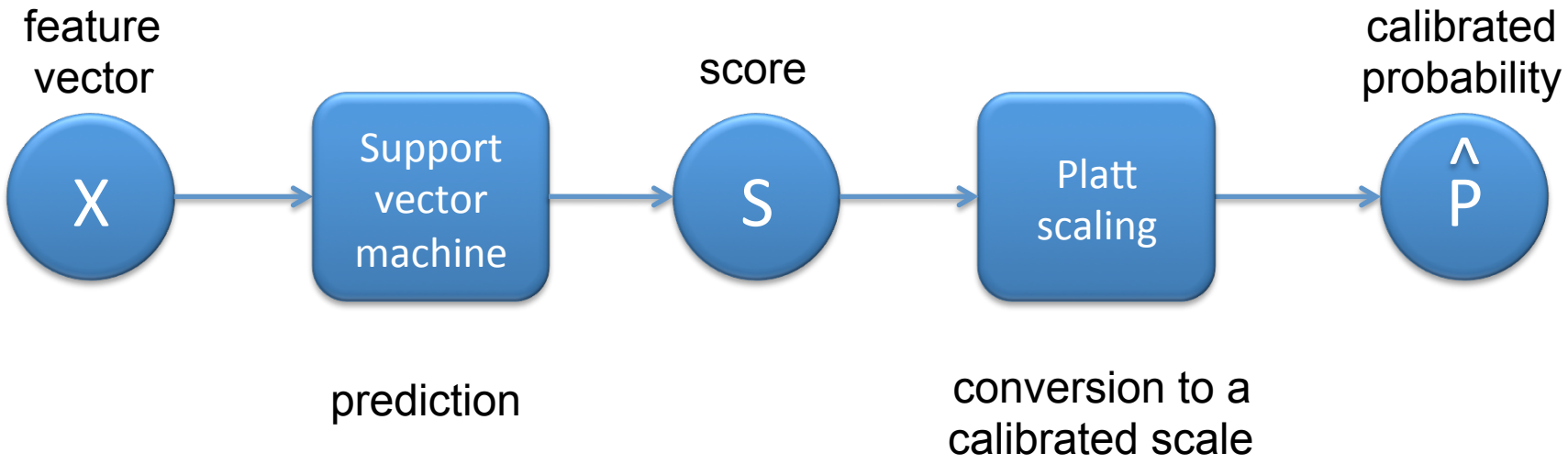
Calibration converts to a meaningful scale



- Calibrated probabilities match with expected frequencies
  - E.g. among $\hat{P}=0.8$ there are 80% positive, 20% negative
  - Calibrated on the training data vs on the test data
- Perfect calibration map: $\hat{P}=P(Y=1|S)$
- Bayes optimal: $\hat{P}=P(Y=1|X)$

Logistic calibration (a.k.a. Platt scaling)

J. Platt (2000). Probabilities for SV machines.
In A. Smola, P. Bartlett, B. Schölkopf, D. Schuurmans (Eds.),
Advances in Large Margin Classifiers, pp.61–74, MIT Press.

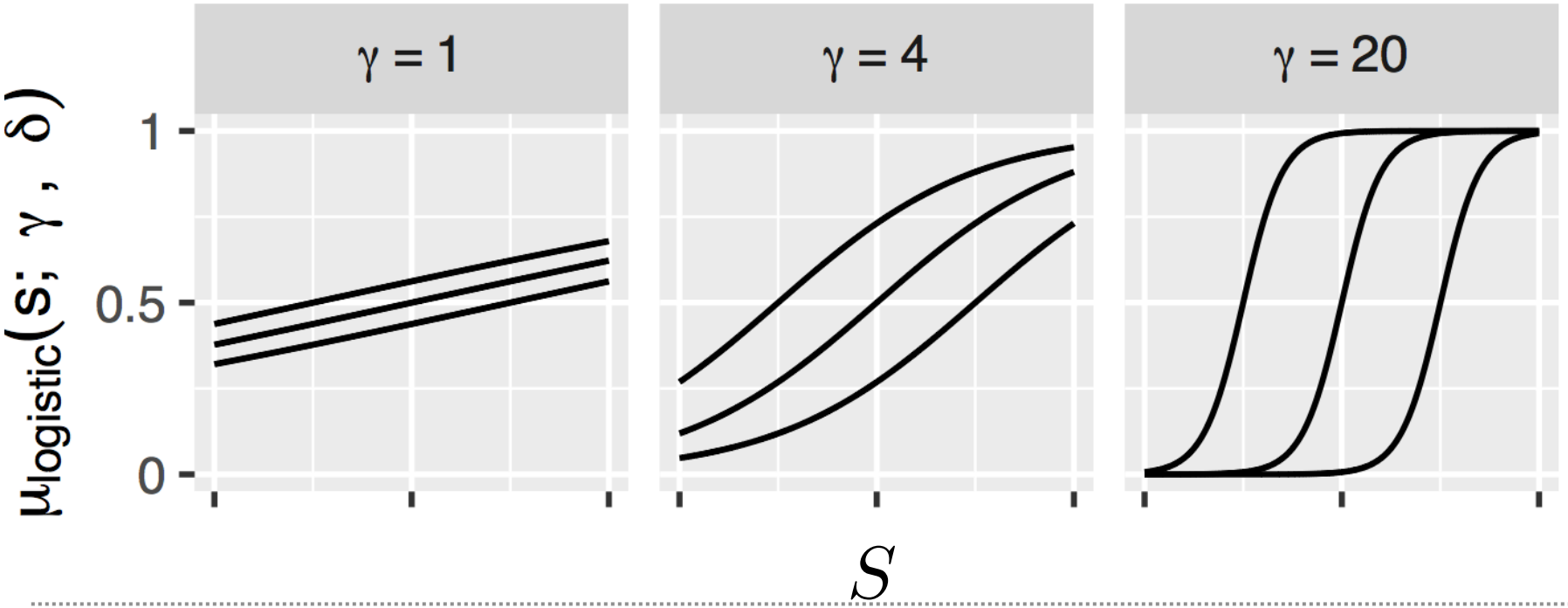


- Logistic sigmoid to convert $[-\infty, +\infty]$ to $[0, 1]$

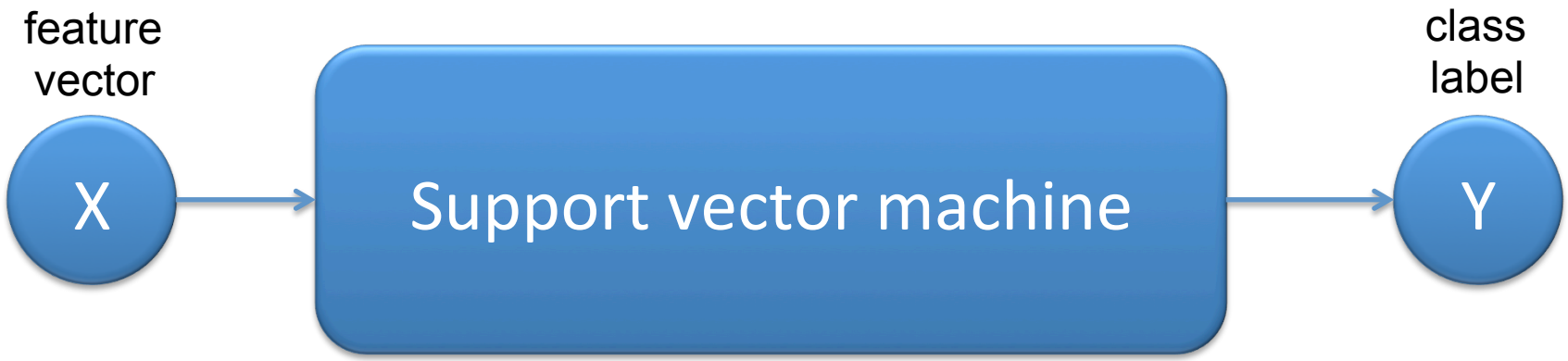
$$\mu_{logistic}(S; \gamma, \delta) = \frac{1}{1 + 1/(\exp(\gamma \cdot S + \delta))}$$

Logistic calibration map family

$$\mu_{logistic}(S;\gamma,\delta) = \frac{1}{1+1/(\exp(\gamma\cdot S+\delta))}$$

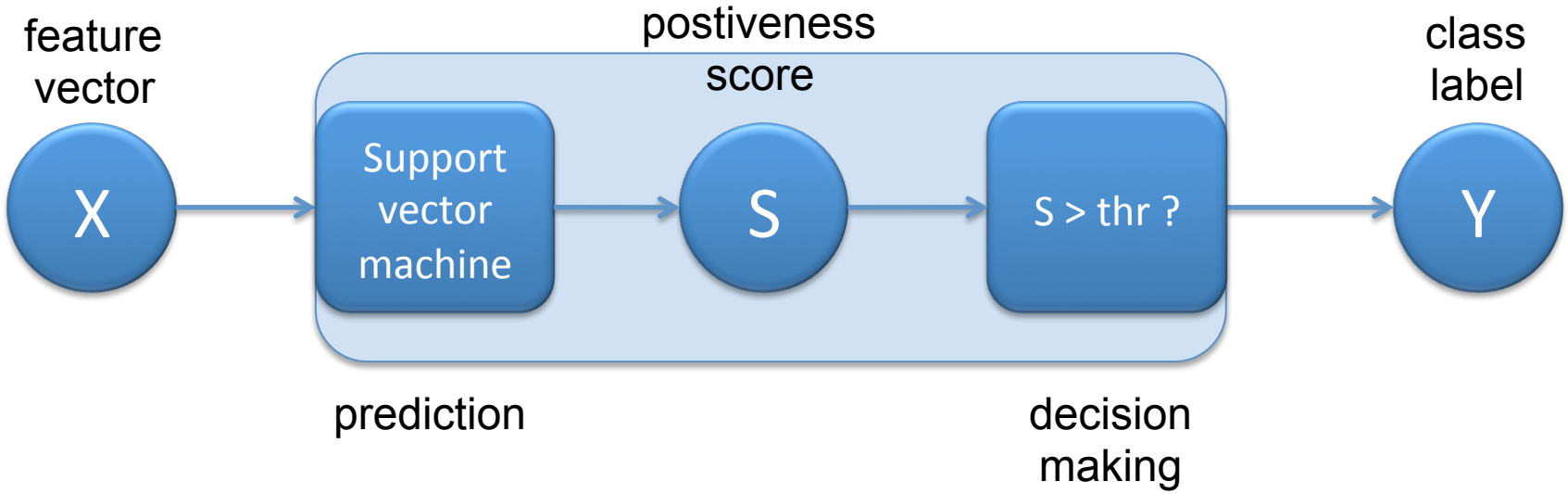


How to fit logistic calibration

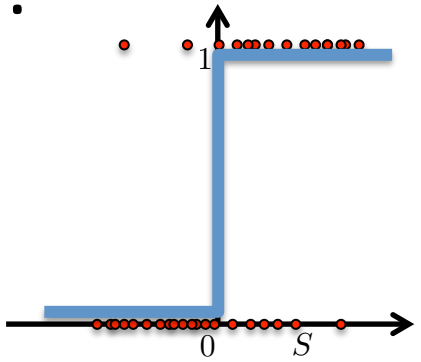


- How to get probabilities from SVM?

How to fit logistic calibration



- How to get probabilities from SVM?
  1. Get the positiveness scores S



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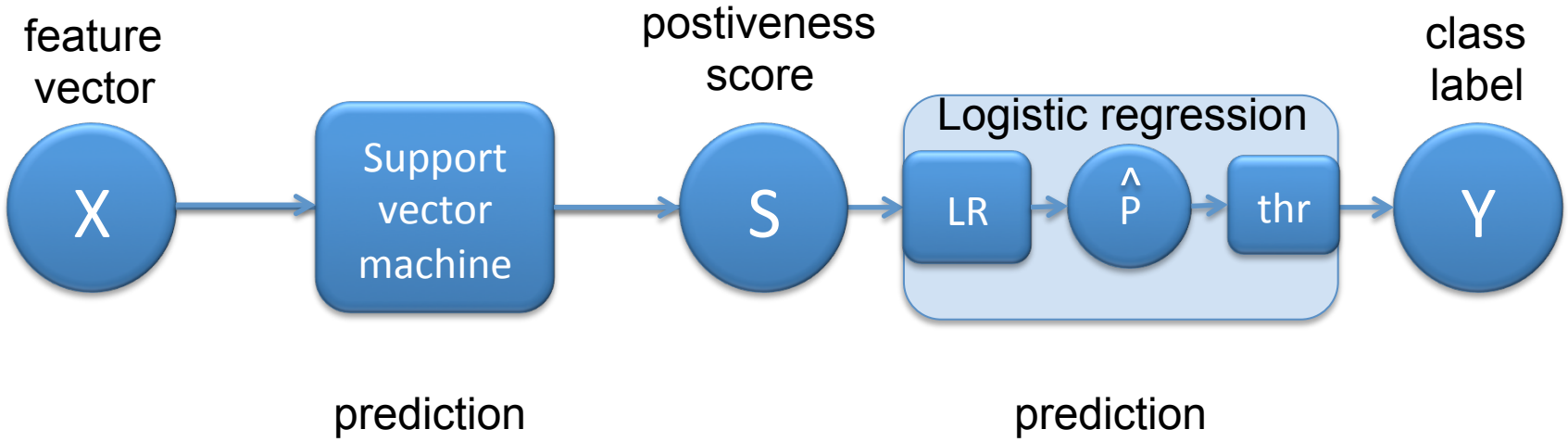
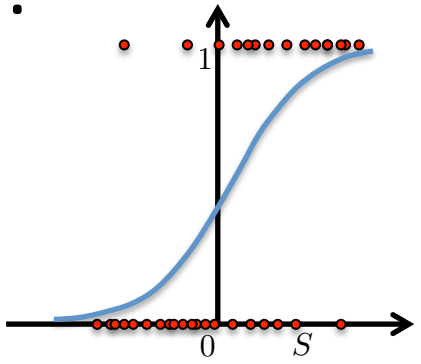


- How to get probabilities from SVM?
  1. Get the positiveness scores S
  2. Replace fixed step function by logistic regression fitting



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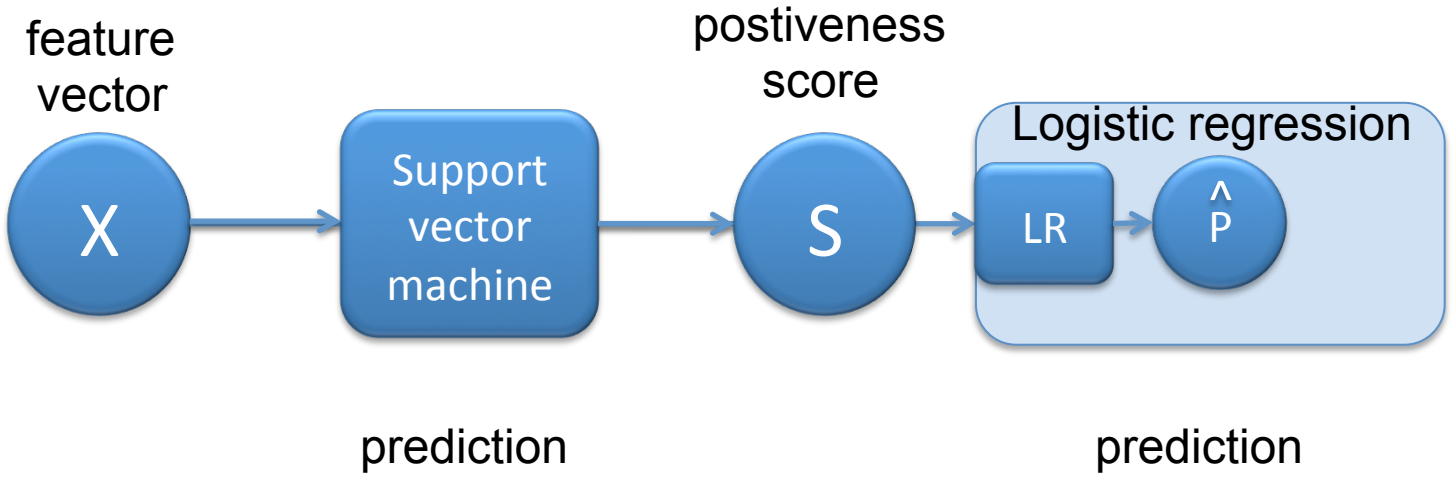

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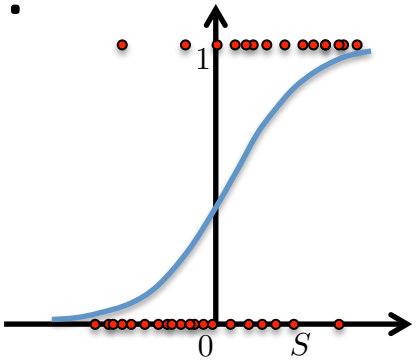

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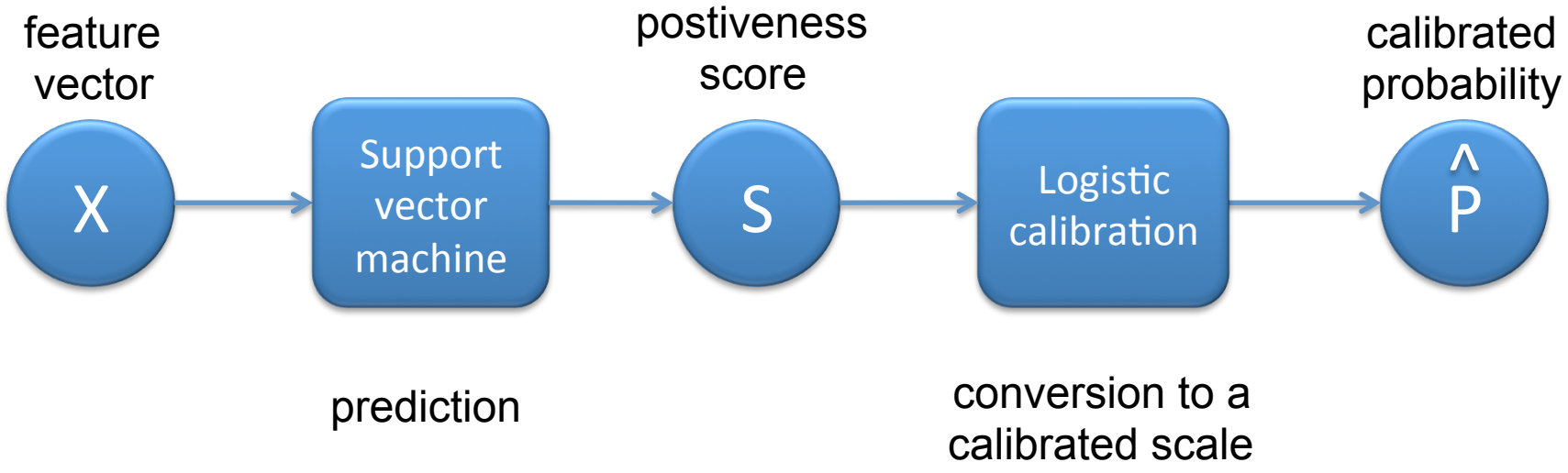

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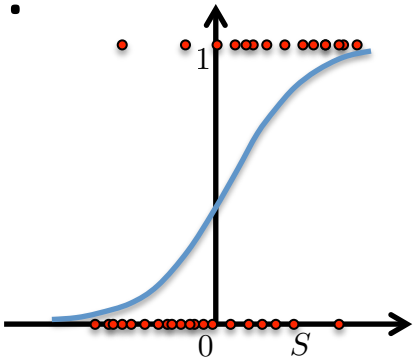
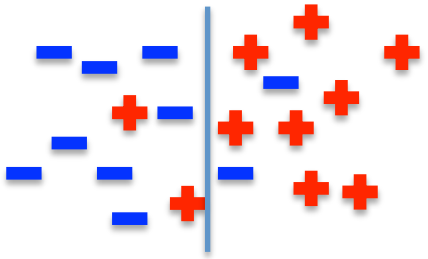
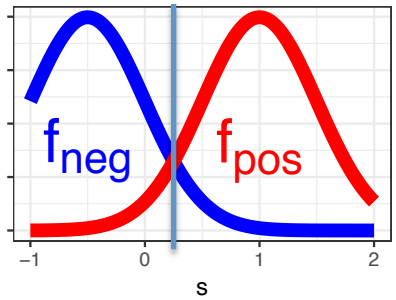


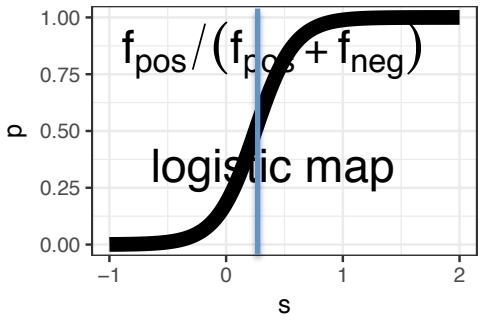
Logistic calibration is perfect if:

- Assume:
  - $p(S \mid Y=+1) \sim \mathcal{N}(\mu_{pos}, \sigma^2)$
  - $p(S \mid Y=-1) \sim \mathcal{N}(\mu_{neg}, \sigma^2)$
  - $p(Y=+1) = p(Y=-1) = 0.5$
- Then:
  - $p(Y=+1 \mid S) = \dfrac{f_{pos}}{f_{pos} + f_{neg}}$

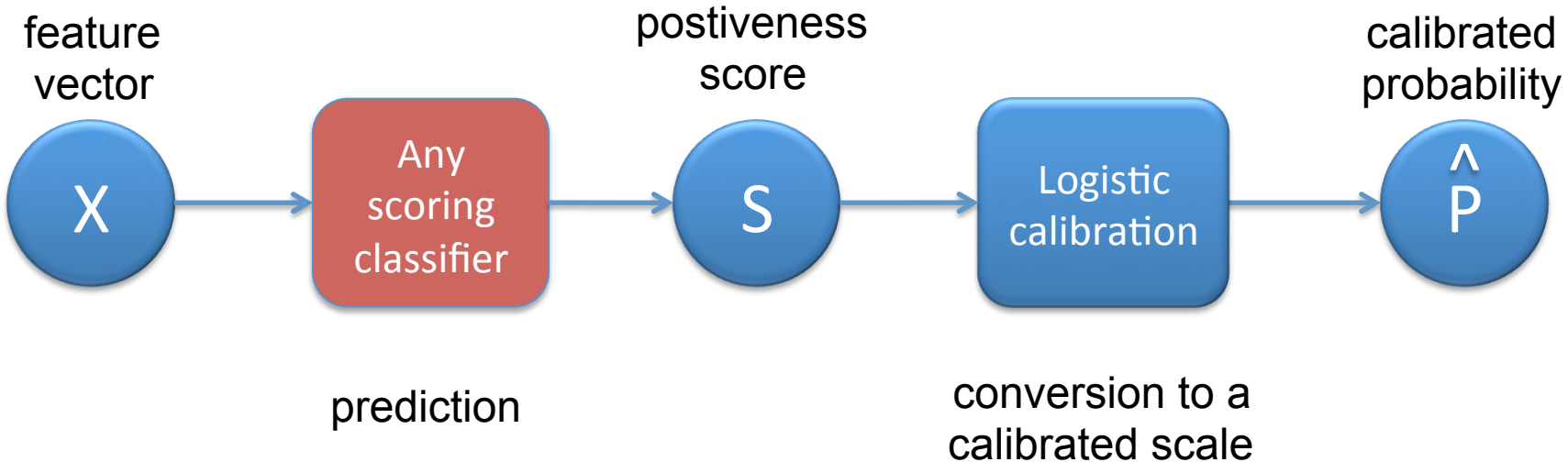
$$= \frac{1}{1 + 1/(\exp(\gamma \cdot S + \delta))}$$





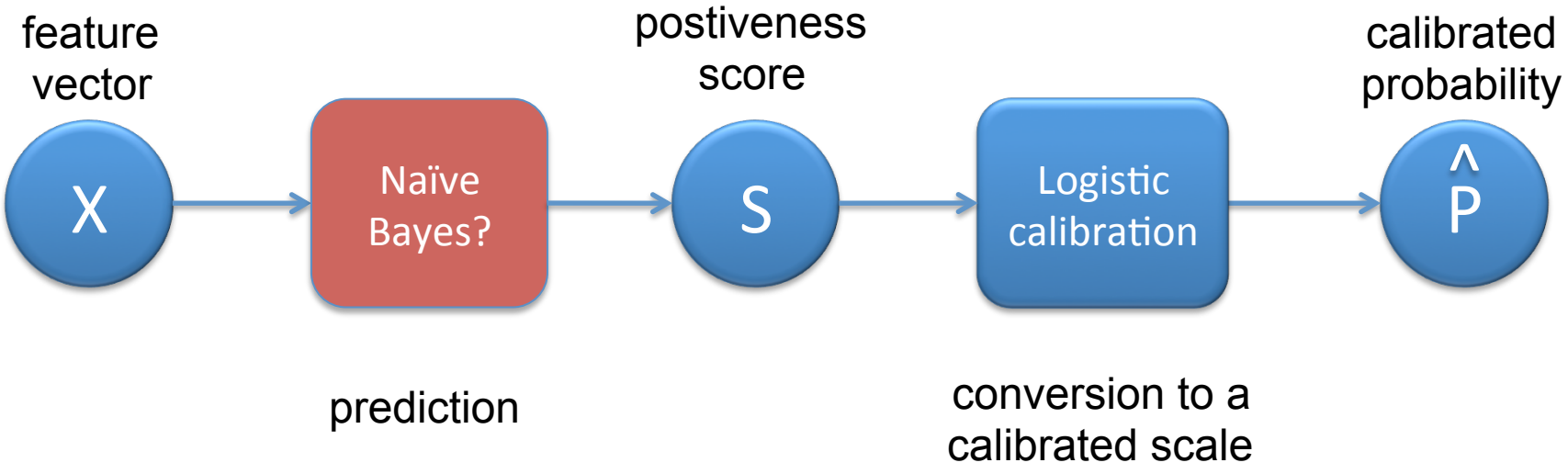


Logistic calibration is widespread

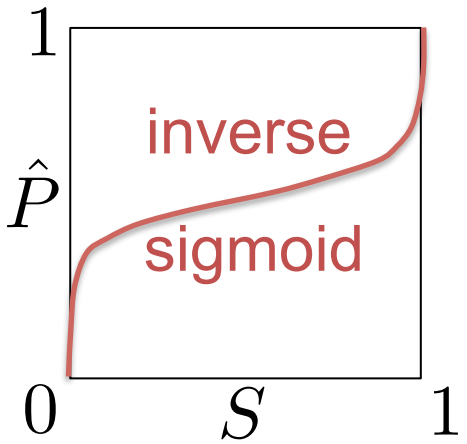


- If scores are already probabilities
  - Then Gaussian assumption questionable

Logistic calibration after Naïve Bayes?



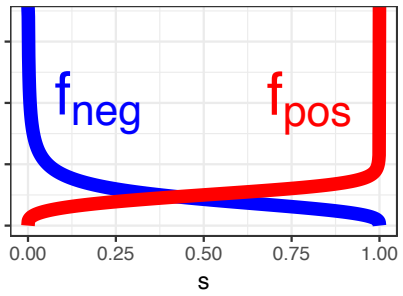
- If scores are already probabilities
  - Then Gaussian assumption questionable
- Naïve Bayes pushes probabilities towards extremes
  - Particularly with many correlated features

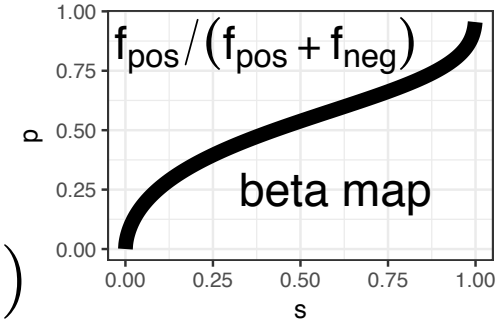


Beta calibration from first principles:

- Assume:
  - $p(S \mid Y=+1) \sim Beta(\alpha_{pos}, \beta_{pos})$
  - $p(S \mid Y=-1) \sim Beta(\alpha_{neg}, \beta_{neg})$
  - $p(Y=+1) = p(Y=-1) = 0.5$
- Then:
  - $p(Y=+1 \mid S) = \dfrac{f_{pos}}{f_{pos} + f_{neg}}$

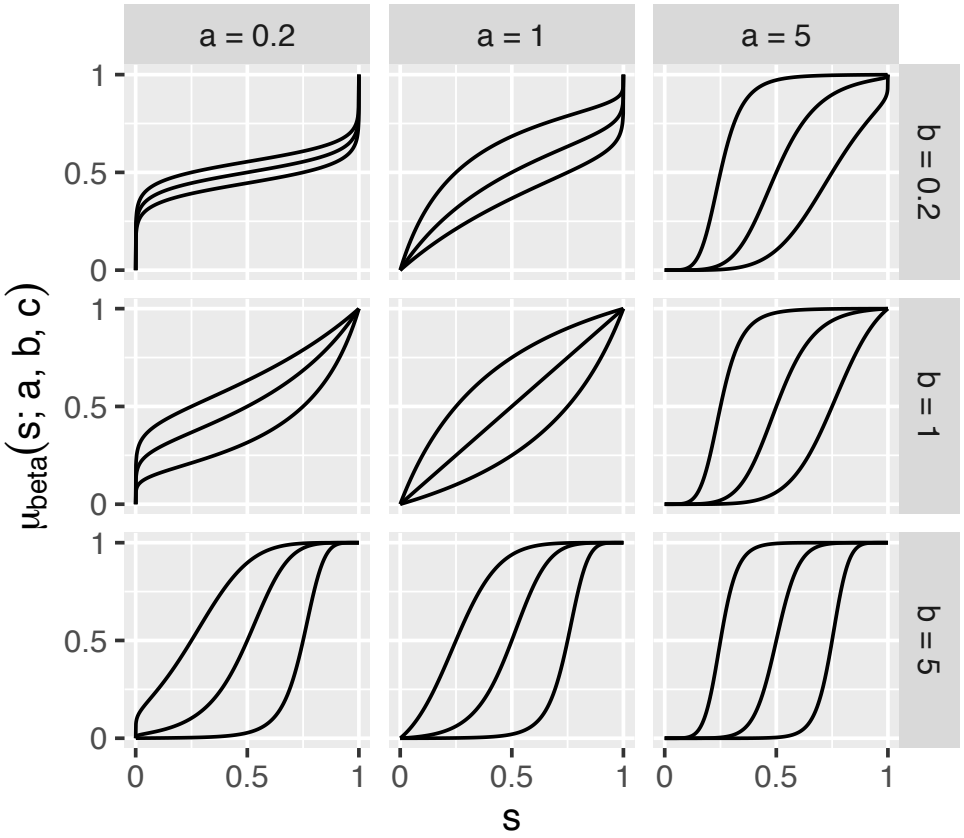
$$= \frac{1}{1 + 1/(e^c \frac{S^a}{(1-S)^b})} =: \mu_{beta}(S; a, b, c)$$





Beta calibration map family

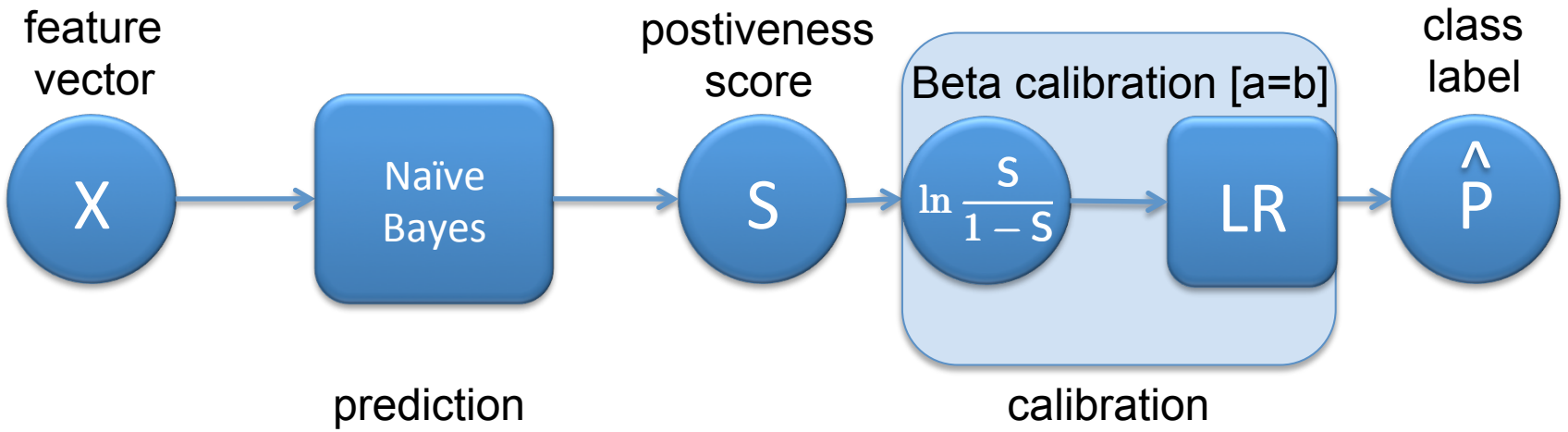
$$\mu_{beta}(S; a, b, c) = \frac{1}{1 + 1/(e^{c}\frac{S^{a}}{(1-S)^{b}})}$$



Logistic calibration vs Beta calibration

$$\mu_{logistic}(S;\gamma,\delta) = \frac{1}{1+1/(\exp(\gamma\cdot S+\delta))} \qquad \mu_{beta}(S;a,b,c) = \frac{1}{1+1/(e^{c}\frac{S^{a}}{(1-S)^{b}})}$$

$$\mu_{logistic}(\ln\frac{S}{1-S};a,c) = \mu_{beta}(S;a,a,c)$$



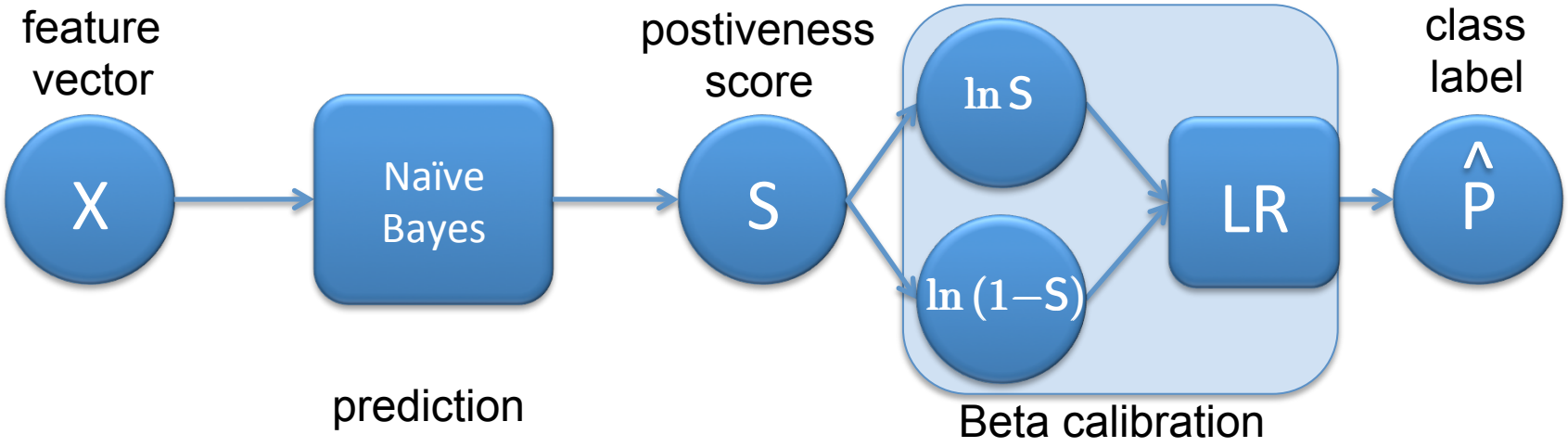
- 2-parameter beta calibration can be implemented as logistic calibration of the log odds

Beta calibration via logistic regression

$$\mu_{logreg}(S', S''; a, b, c) = \frac{1}{1 + 1/(\exp(a \cdot S' + b \cdot S'' + c))}$$

$$\mu_{beta}(S; a, b, c) = \frac{1}{1 + 1/(e^c \frac{S^a}{(1-S)^b})}$$

$$\mu_{logreg}(\ln S, -\ln(1-S); a, b, c) = \mu_{beta}(S; a, b, c)$$



- 3-parameter beta calibration can be implemented as logistic regression on features $\ln S$ and $\ln(1-S)$

Experimental setup

- 41 UCI datasets
- 10x5-fold cross-validation
- Calibration with 3-fold internal cross-validation, predictions averaged [same as Platt 2000]
- Models:
  - NB : Naïve Bayes
  - Ada-O : Adaboost original
  - Ada-S : Adaboost in Scikit (SAMME)
- Evaluation measures: proper scoring rules
  - Brier score (squared error) $BS = \mathbb{E}[(\hat{P} - \mathbb{1}_{Y=1})^2]$
  - Log-loss (cross-entropy) $LL = \mathbb{E}[-\ln(\hat{P})\,\mathbb{1}_{Y=1} - \ln(1-\hat{P})\,\mathbb{1}_{Y=-1}]$

Results (Adaboost-original, log-loss)

Table 2: Log-loss results with Ada-O classifier. Best results are marked in **bold** and subscripts indicate the ranks (before rounding to 3 decimal digits).

dataset	uncalibrated	beta	isotonic	logistic
abalone	0.612_2	$\mathbf{0.612}_1$	0.626_4	0.614_3
autos	0.427_4	$\mathbf{0.283}_1$	0.416_3	0.287_2
balance	0.049_4	$\mathbf{0.037}_1$	0.041_3	0.038_2
car	0.114_2	$\mathbf{0.109}_1$	0.122_4	0.119_3
clevela	0.496_3	$\mathbf{0.417}_1$	0.523_4	0.429_2
credit-	0.360_3	0.341_2	0.444_4	$\mathbf{0.338}_1$
dermato	0.036_4	$\mathbf{0.019}_1$	0.035_3	0.021_2
diabete	0.506_3	$\mathbf{0.484}_1$	0.525_4	0.495_2
ecoli	0.326_4	$\mathbf{0.145}_1$	0.224_3	0.159_2
flare	$\mathbf{0.404}_1$	0.404_2	0.421_4	0.408_3
german	0.511_3	0.506_2	0.538_4	$\mathbf{0.506}_1$
glass	0.696_4	0.489_2	0.560_3	$\mathbf{0.485}_1$
heart-s	0.570_4	$\mathbf{0.427}_1$	0.557_3	0.443_2
hepatit	0.805_4	$\mathbf{0.392}_1$	0.431_3	0.411_2
horse	0.642_4	$\mathbf{0.413}_1$	0.524_3	0.418_2
ionosph	0.381_4	$\mathbf{0.203}_1$	0.296_3	0.227_2
iris	0.127_4	0.000_2	$\mathbf{0.000}_1$	0.000_3
landsat	0.041_2	$\mathbf{0.040}_1$	0.043_3	0.053_4
letter	0.037_3	0.035_2	$\mathbf{0.035}_1$	0.044_4
libras-	0.589_4	$\mathbf{0.100}_1$	0.184_3	0.112_2
lung-ca	0.193_4	$\mathbf{0.139}_1$	0.189_3	0.139_2
mfeat-k	0.062_4	$\mathbf{0.027}_1$	0.048_3	0.032_2
mfeat-m	0.040_4	$\mathbf{0.014}_1$	0.026_3	0.014_2
mfeat-z	0.095_4	$\mathbf{0.032}_1$	0.063_3	0.039_2
mushroo	0.000_4	0.000_3	0.000_2	$\mathbf{0.000}_1$
optdigi	0.035_2	$\mathbf{0.033}_1$	0.044_4	0.040_3
page-bl	0.093_2	$\mathbf{0.089}_1$	0.098_3	0.109_4
pendigi	0.017_2	$\mathbf{0.017}_1$	0.023_4	0.021_3
scene-c	0.384_4	$\mathbf{0.364}_1$	0.376_2	0.378_3
segment	0.020_3	$\mathbf{0.010}_1$	0.023_4	0.013_2
shuttle	0.000_2	$\mathbf{0.000}_1$	0.001_4	0.000_3
sonar	0.941_4	$\mathbf{0.404}_1$	0.486_3	0.440_2
spambas	0.162_2	$\mathbf{0.162}_1$	0.173_4	0.167_3
tic-tac	0.379_4	$\mathbf{0.333}_1$	0.340_3	0.339_2
vehicle	0.077_2	$\mathbf{0.068}_1$	0.131_4	0.077_3
vowel	0.076_2	$\mathbf{0.071}_1$	0.094_4	0.085_3
wavefor	0.253_2	$\mathbf{0.252}_1$	0.264_3	0.271_4
wdbc	0.256_4	$\mathbf{0.089}_1$	0.141_3	0.107_2
wpbc	1.016_4	0.500_2	$\mathbf{0.496}_1$	0.503_3
yeast	0.510_2	$\mathbf{0.509}_1$	0.543_4	0.514_3
zoo	0.132_4	0.013_3	$\mathbf{0.013}_1$	0.013_2
rank	3.20	1.27	3.12	2.41

Key findings

- Beta calibration better than logistic calibration:

	Naïve Bayes	Adaboost-O	Adaboost-S
Brier score	++	++	+
Log-loss	++	++	+

- Beta calibration better than isotonic calibration in log-loss:

	Naïve Bayes	Adaboost-O	Adaboost-S
Brier score	+	+	-
Log-loss	++	++	++

- Full 3-parameter version better than 2-parameter versions (but often non-significantly)

Availability

- https://betacal.github.io
  - Python package
  - R package
- Or, implement your own as logistic regression on the dataset with two features: $\ln s$ and $\ln(1-s)$

Next: Dirichlet calibration for multi-class

- Dirichlet distribution is the multi-class generalisation of beta distribution
- Beta calibration can also be generalised in a relatively straight-forward manner
- https://dircal.github.io (paper in preparation)
- Or, implement yourself as logistic regression on features $\ln p_1, \ln p_2, \ldots, \ln p_k$ where k is the number of classes

Summary

- Scoring classifiers
  - Allow for separation of prediction and decision making
- Calibrated probabilities
  - Provide a standard scale of scores
- Logistic calibration
  - Is perfect when score conditional densities are Gaussian
- Beta calibration
  - Is perfect when score conditional densities are Beta
- Beta calibration improves logistic calibration if scores are in [0,1] range :
  - Well-founded, easily implemented, better performance
  - https://betacal.github.io