Statistical Methods for High-dimensional Biology

STAT 540

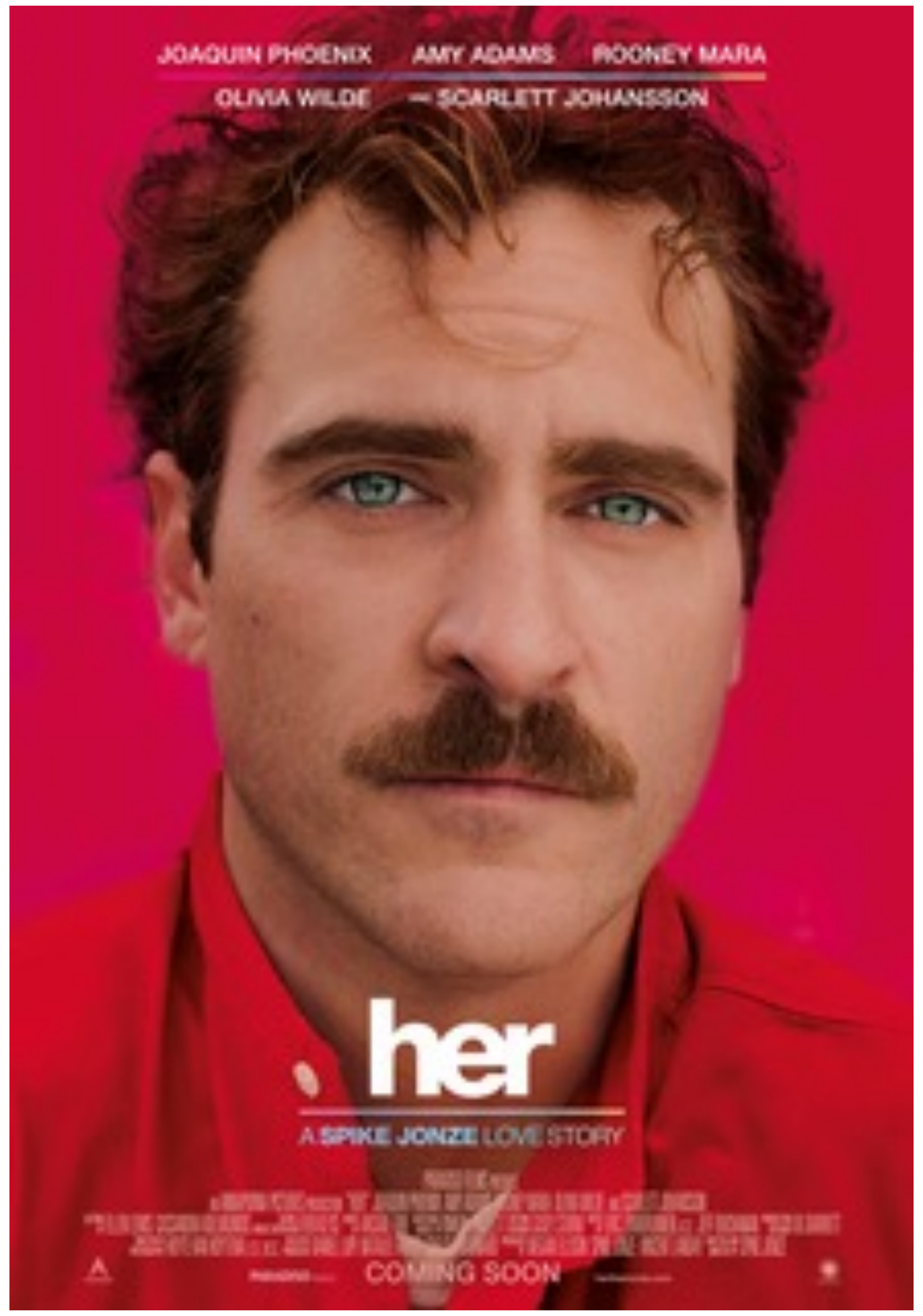
Supervised Learning I

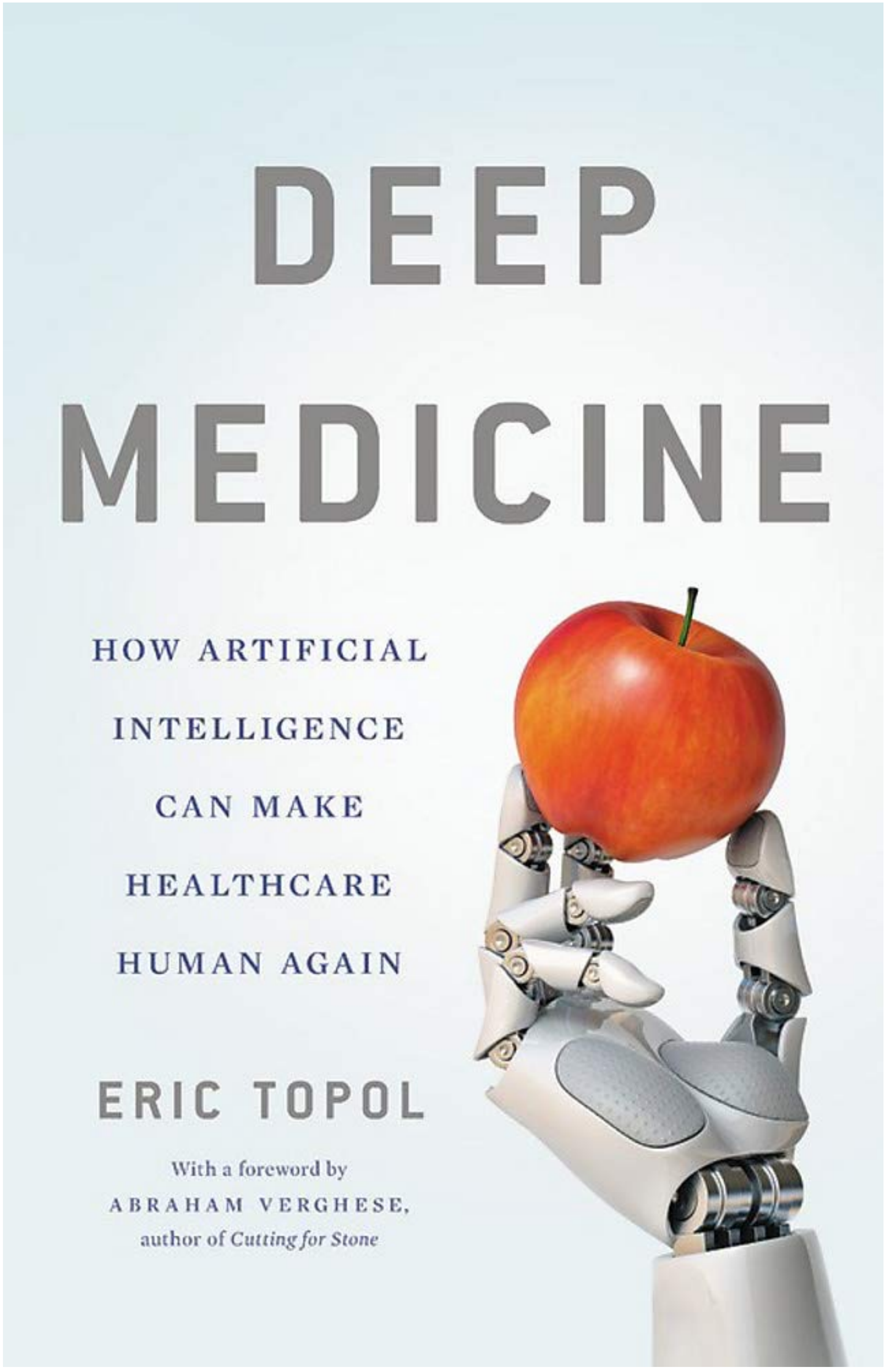
Yongjin Park, UBC Path&Lab, STAT, BC Cancer

Today's lecture

- **A Brief History of Machine Learning in Computational Biology**
  - What is AI/ML? Why ML in Comp. Bio?
  - AI/ML in many OMICs problems
- **Supervised Statistical Learning 101**
  - Binary classification problem
  - Cell-type deconvolution example
  - Discriminative vs. Generative learning
- **Evaluation metrics**

What is ML or AI? Is it Hype?





Strong AI

AI in medicine

Keep calm, just keep on training

Strong AI

data

TensorFlow

PyTorch

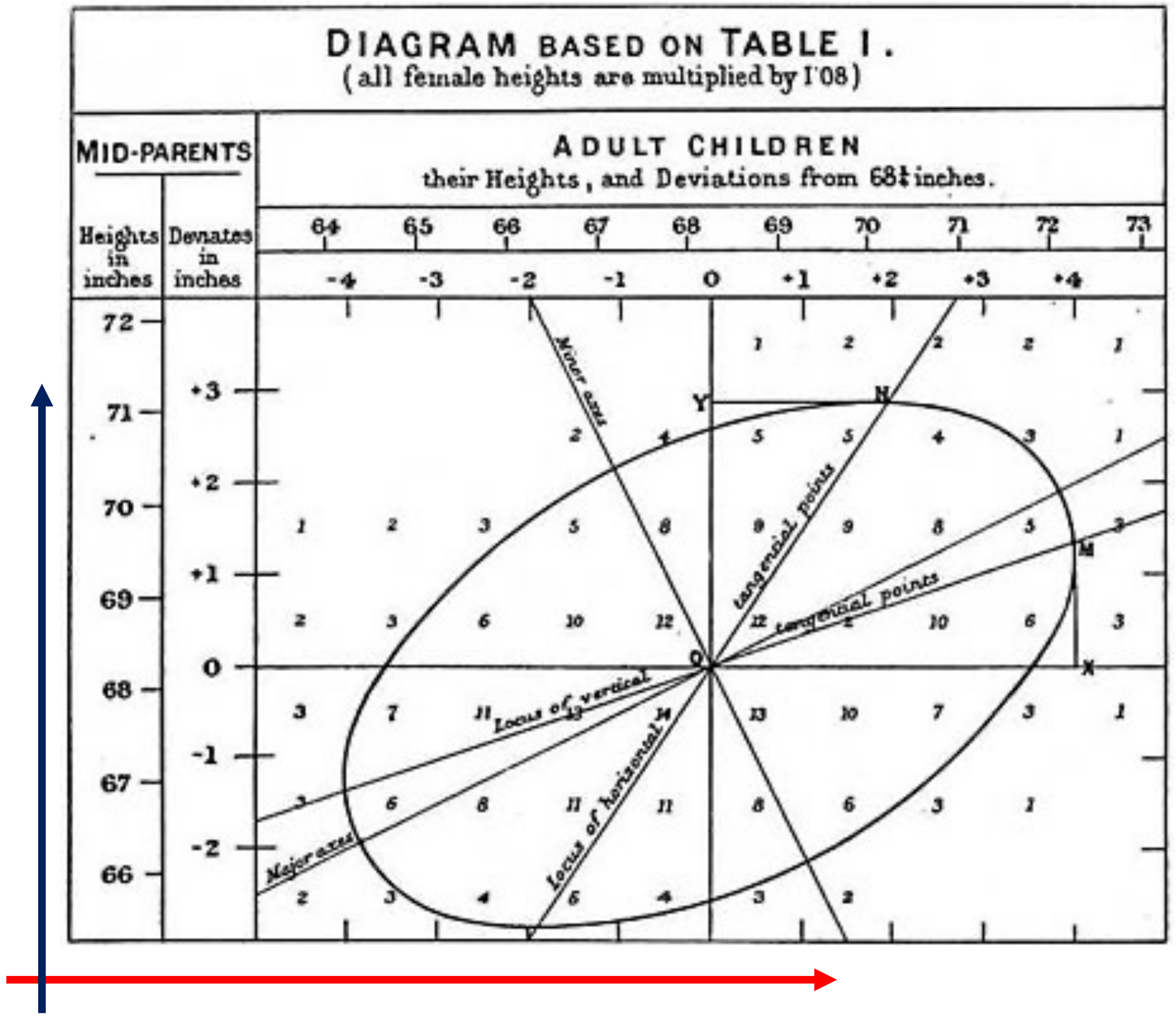
math +
engineering
(function)

f(x)

Weak AI ≈ Machine Learning ≈
Statistical Learning ≈
Intelligence Augmentation

Is it the very first example of statistical learning?

How tall is your parent? (x)

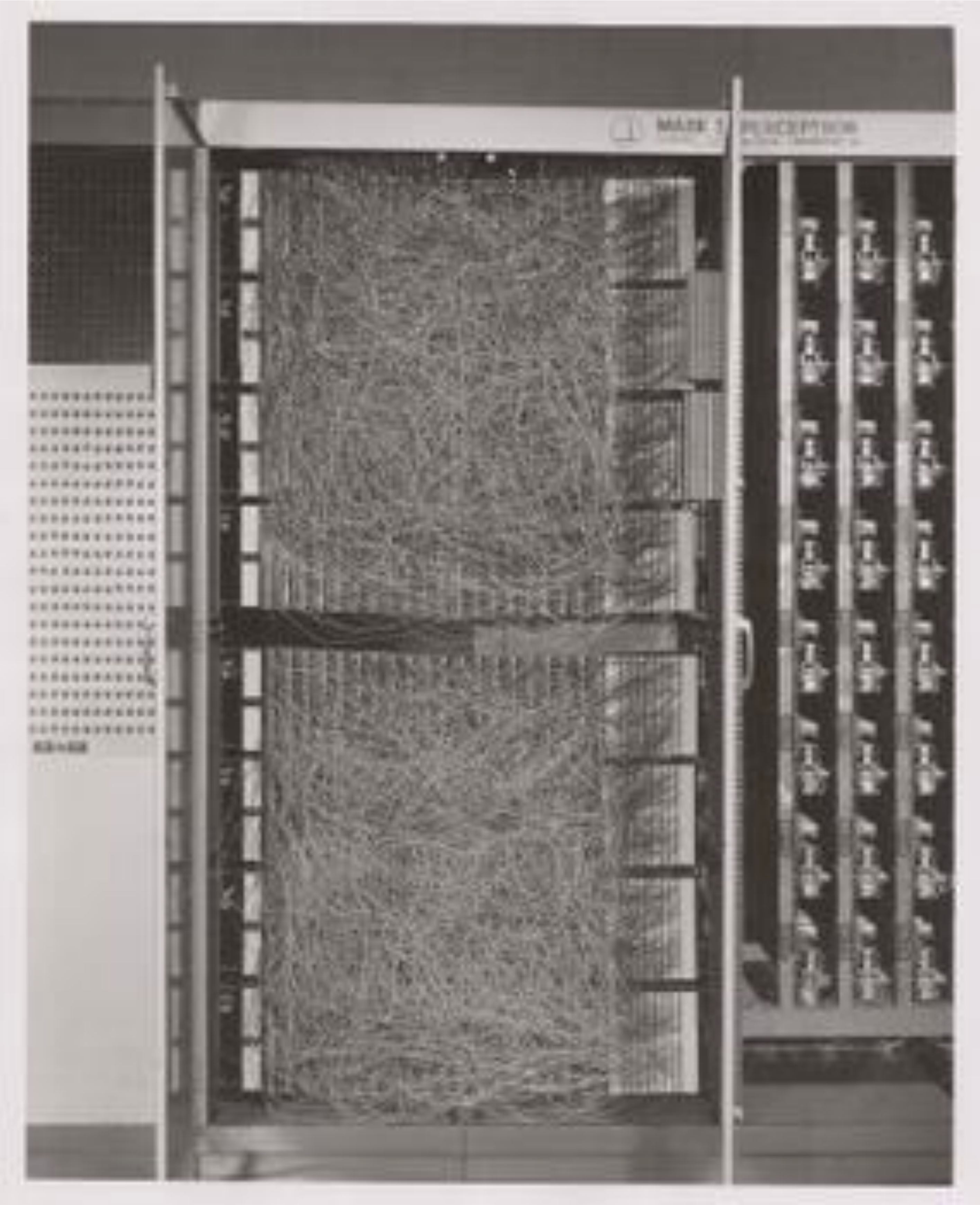


How tall are you? (y)

Galton's 1886 "regression toward the mean"

$$y \sim f(x)$$

Programming how to learn in computer

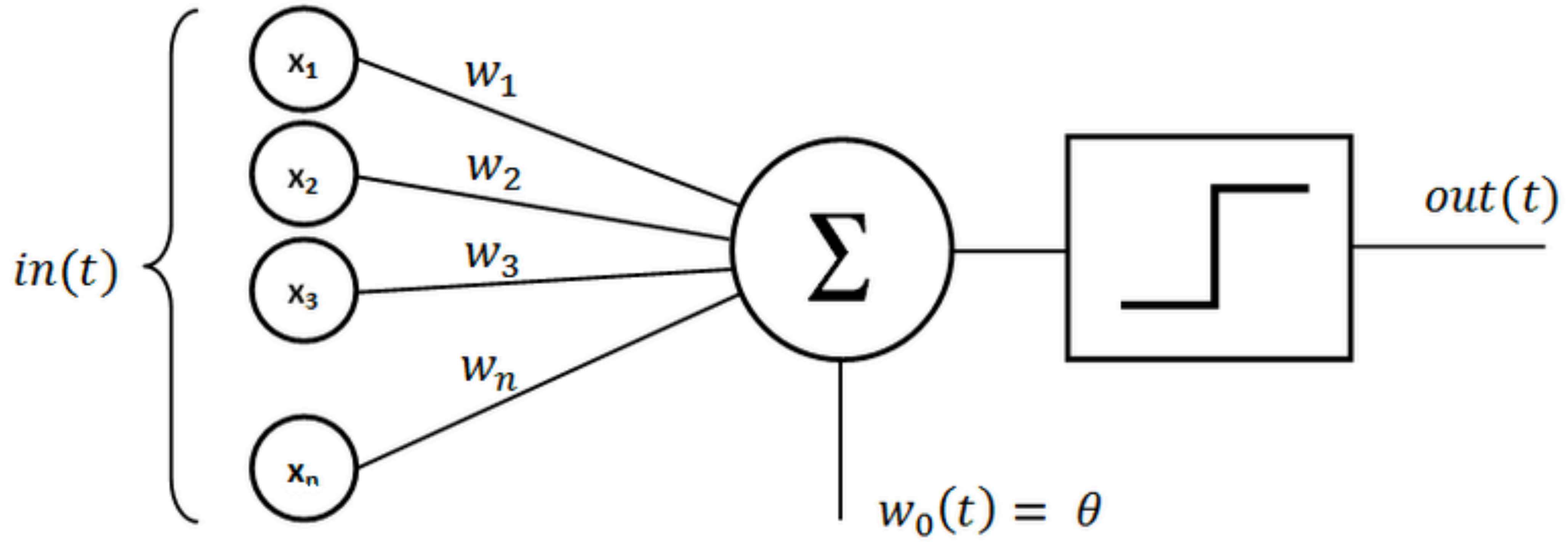


Psychological Review
Vol. 65, No. 6, 1958

THE PERCEPTRON: A PROBABILISTIC MODEL FOR INFORMATION STORAGE AND ORGANIZATION IN THE BRAIN[1]

F. ROSENBLATT

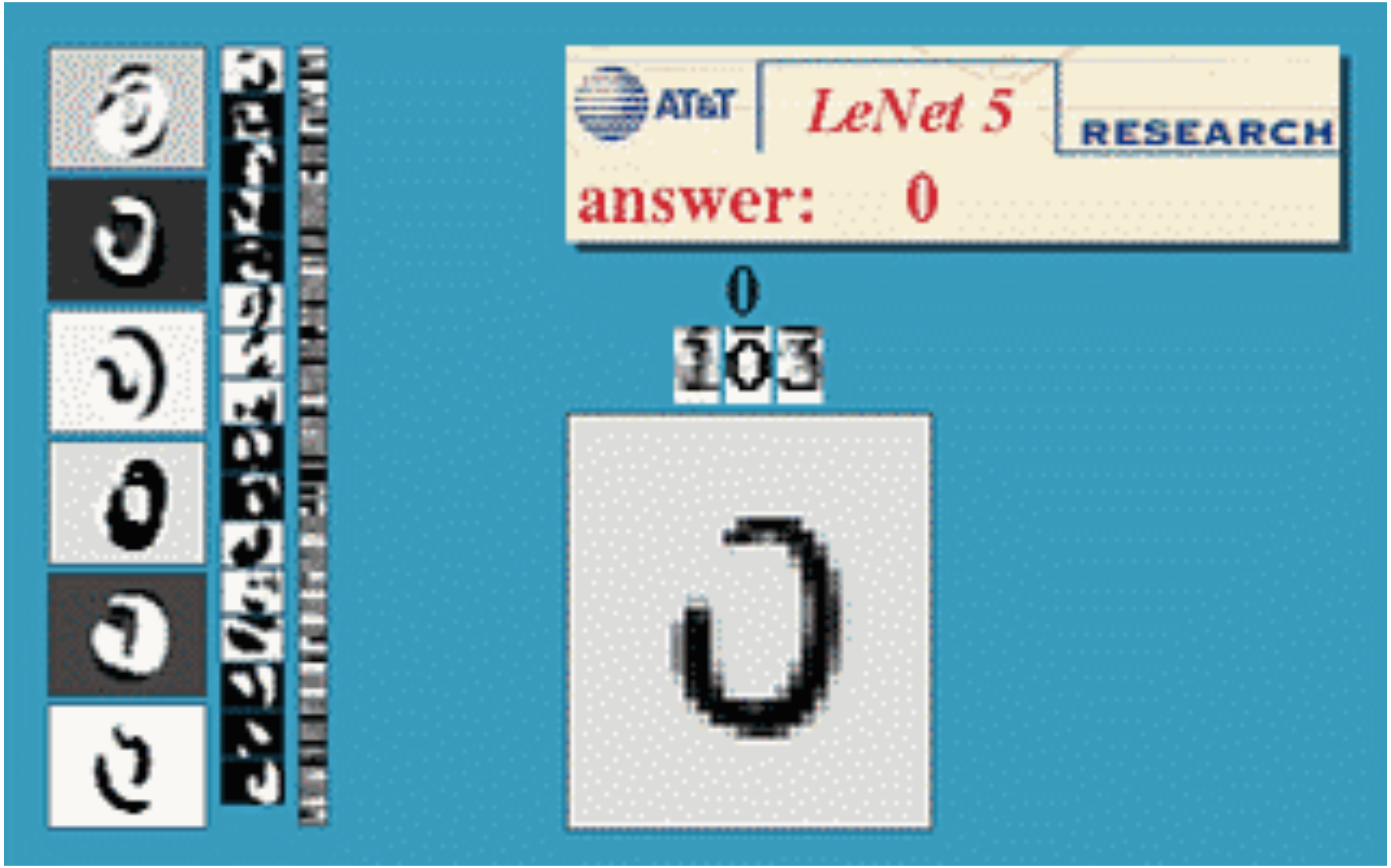
Cornell Aeronautical Laboratory



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

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

Yann Lecun’s Convolutional Neural Network



http://yann.lecun.com/exdb/lenet/

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

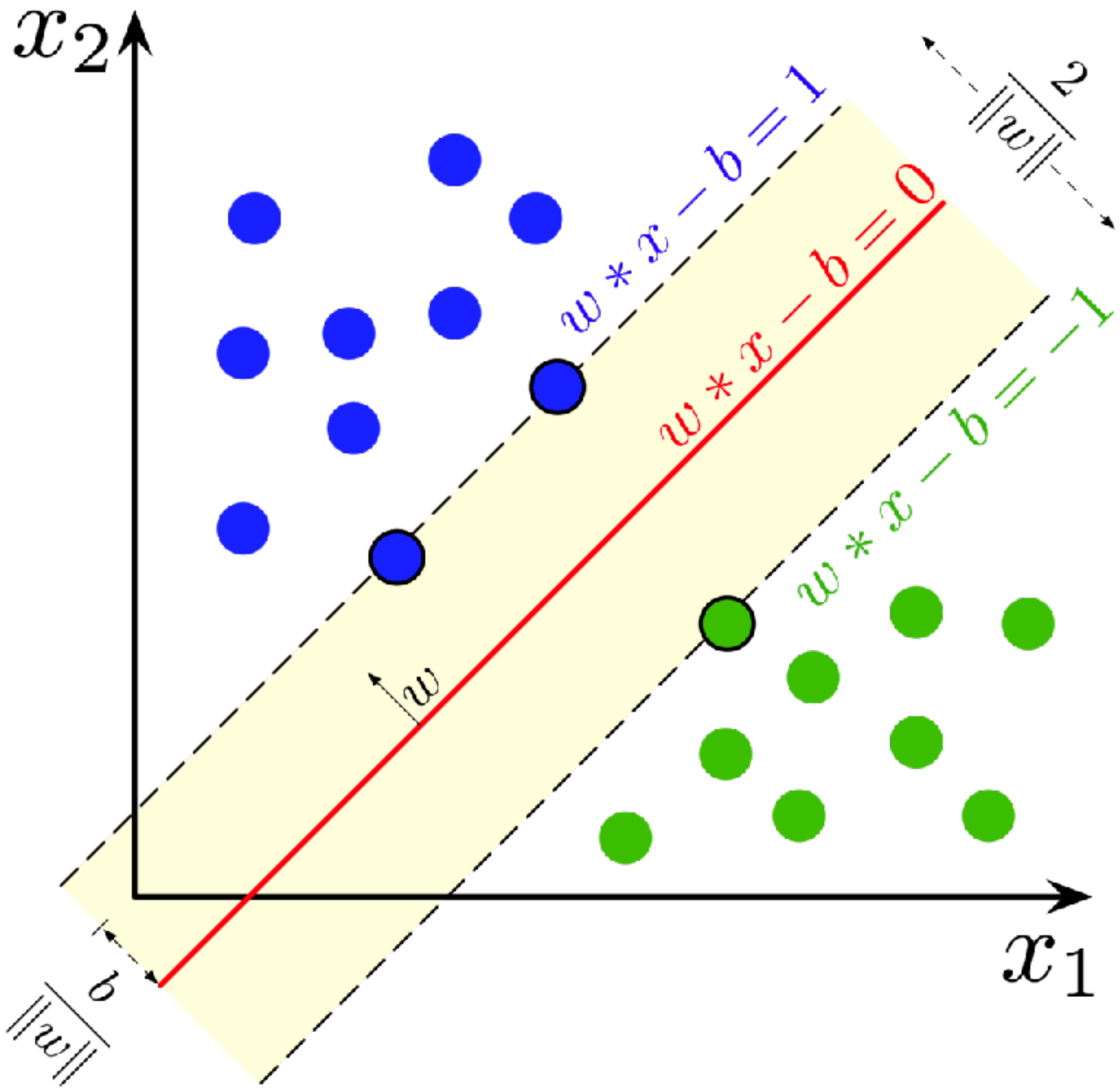
AI/ML: Data-driven innovations

28 x 28 pixel

Yann LeCunn, 1998

The MNIST digits

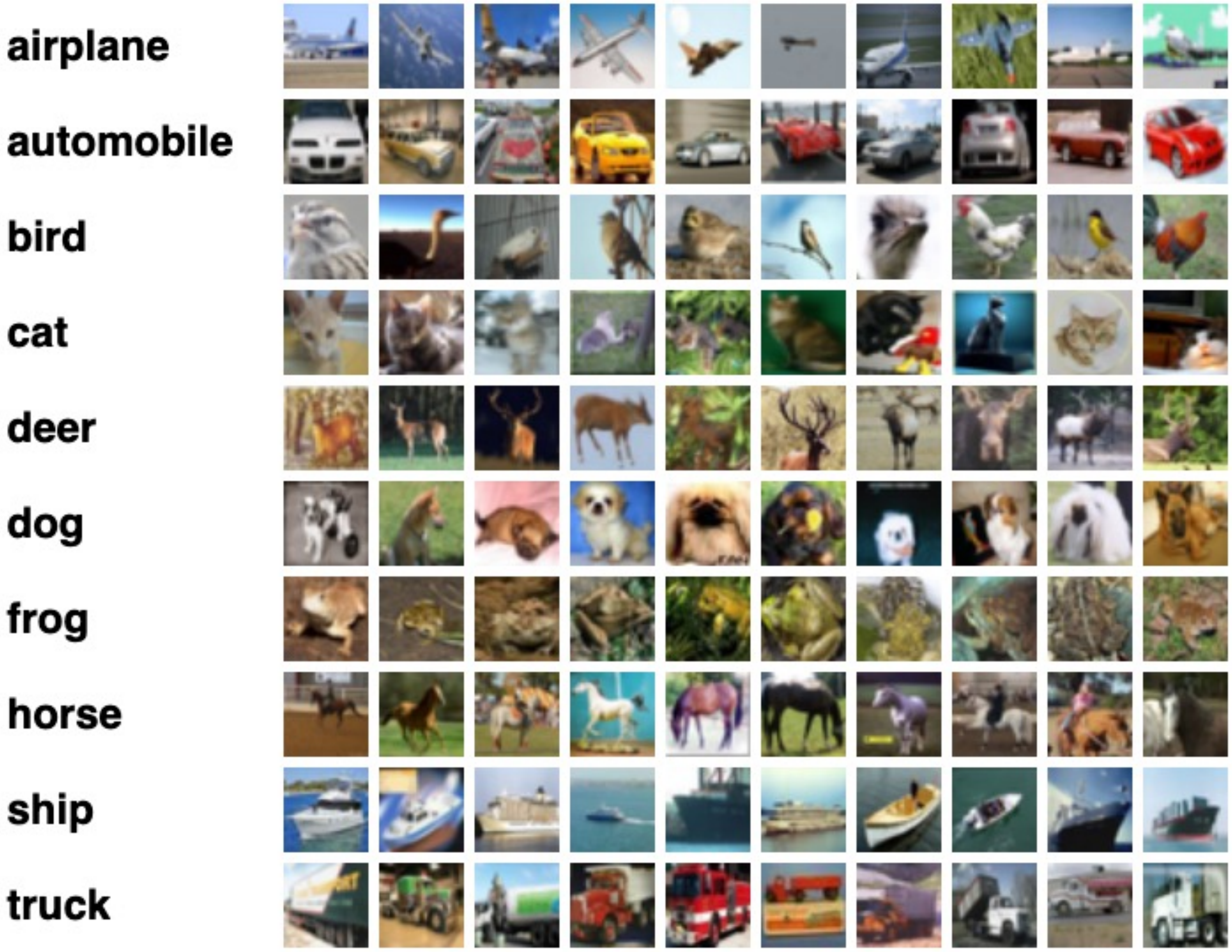
Support vector machine (Vladimir Vapnik)



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

https://www.facebook.com/MetaAI/photos/a.352980534878906/1177827992394152/

AI/ML: Data-driven innovations

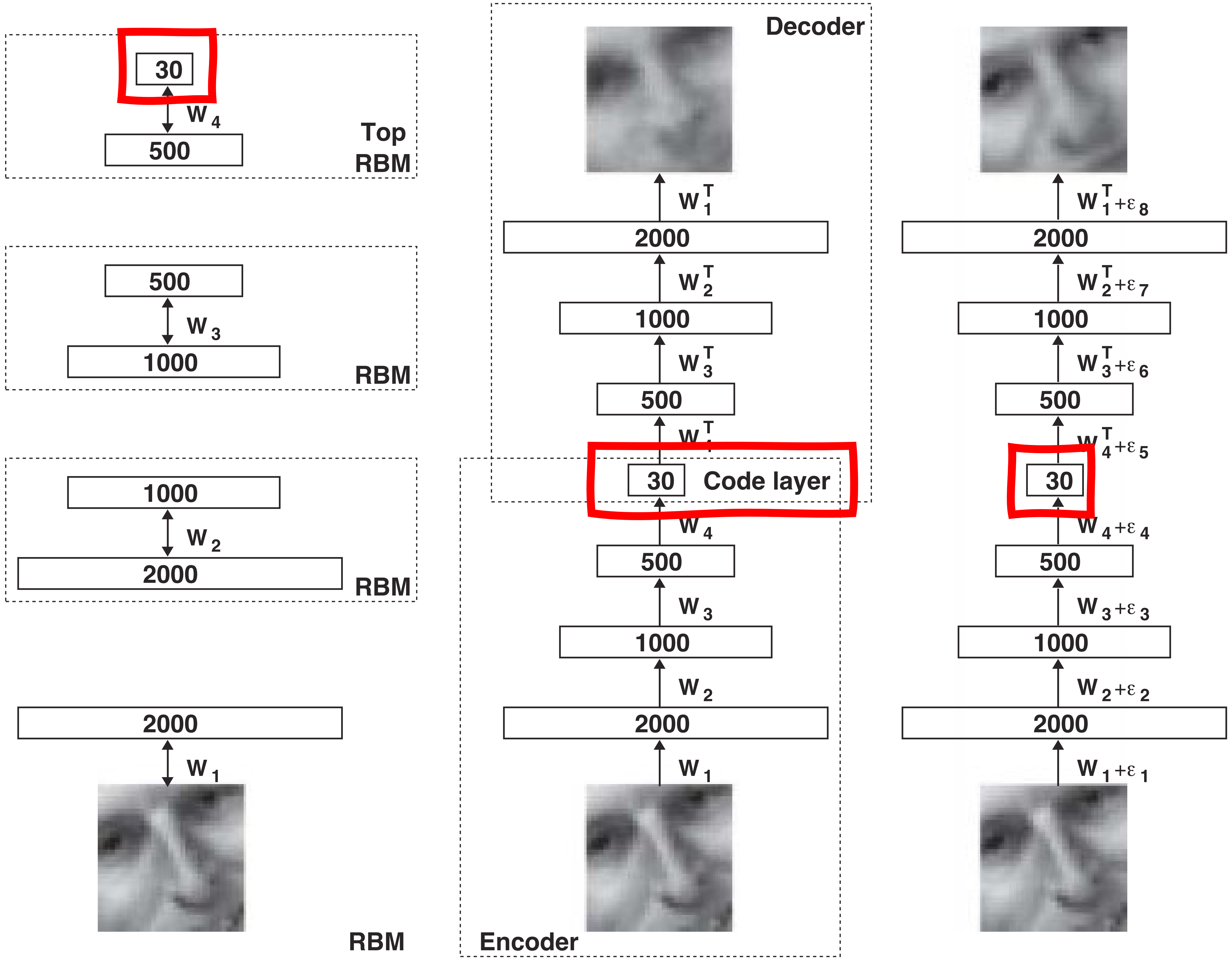


The CIFAR-10

32 x 32 images

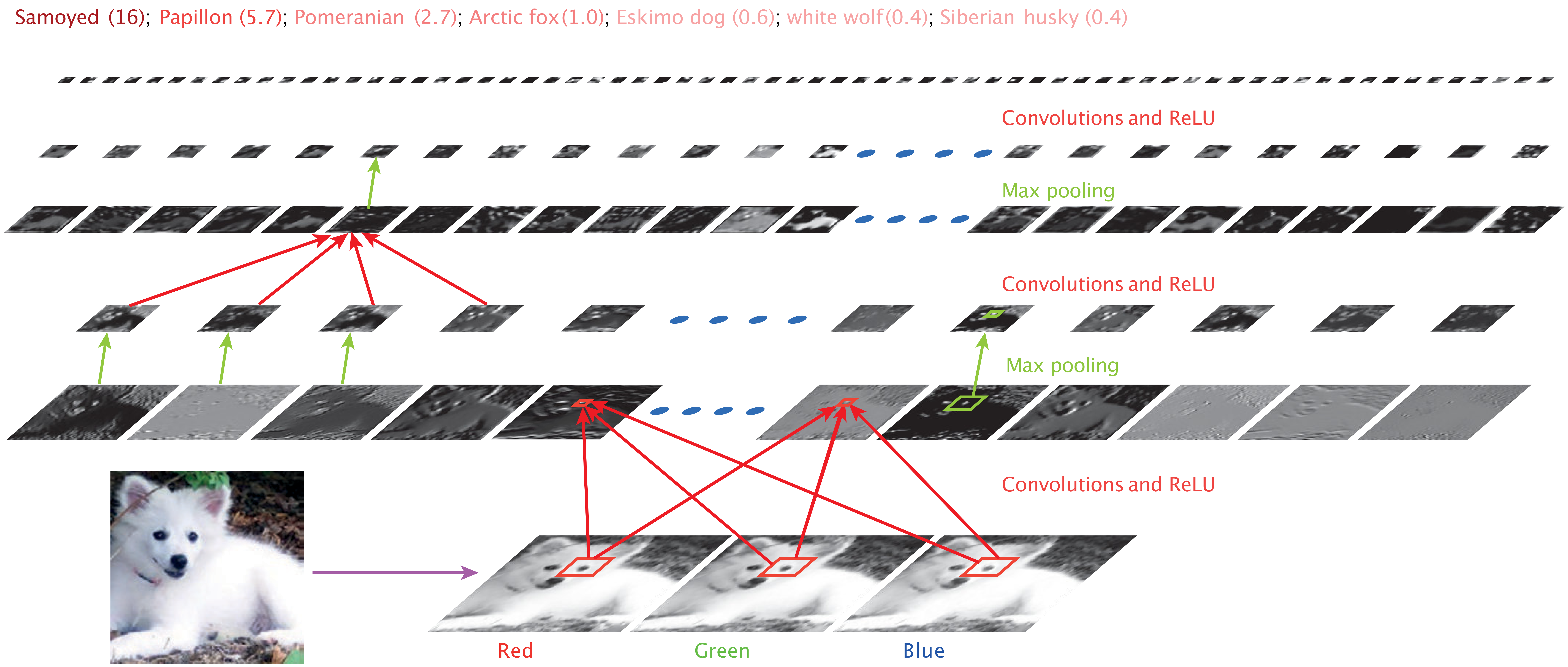
Alex Krizhevsky, 2009

Classic examples: Deep learning models



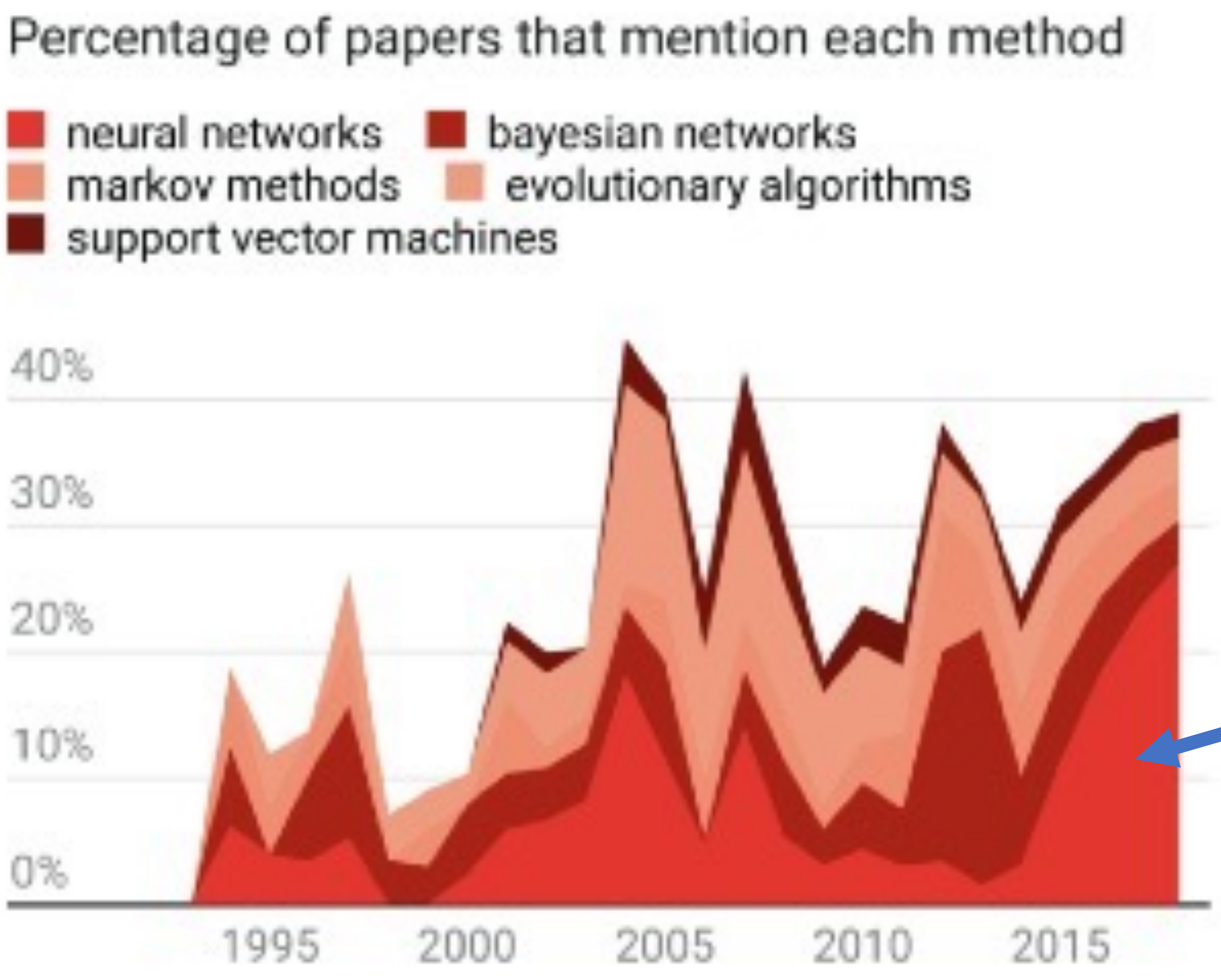
Hinton and Salakhutdinov, Science (2006)

Classic examples: Conv. Neural Networks



LeCun, Bengio, Hinton, *Nature* (2015)

AI/ML in 2021 ≈ mostly Neural Networks



Data from 16,625 papers from arXiv

Neural Networks!
(trained on millions
of samples)

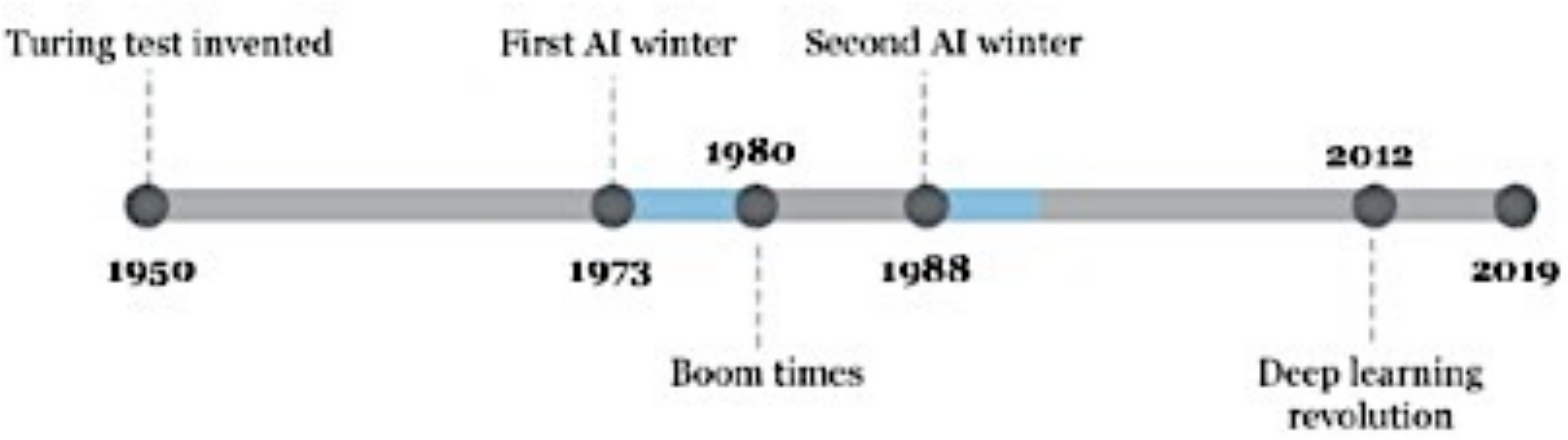
Analyzing the Prospect of an Approaching AI Winter

Schuchmann (2019)

What is this image?

https://theconversation.com/what-is-a-neural-network-a-computer-scientist-explains-151897

Big data: difference between now & then



N <1k N >1M

Schuchmann (2019)

https://blogs.nvidia.com/blog/2019/08/21/drive-labs-autonomous-vehicle-ride/

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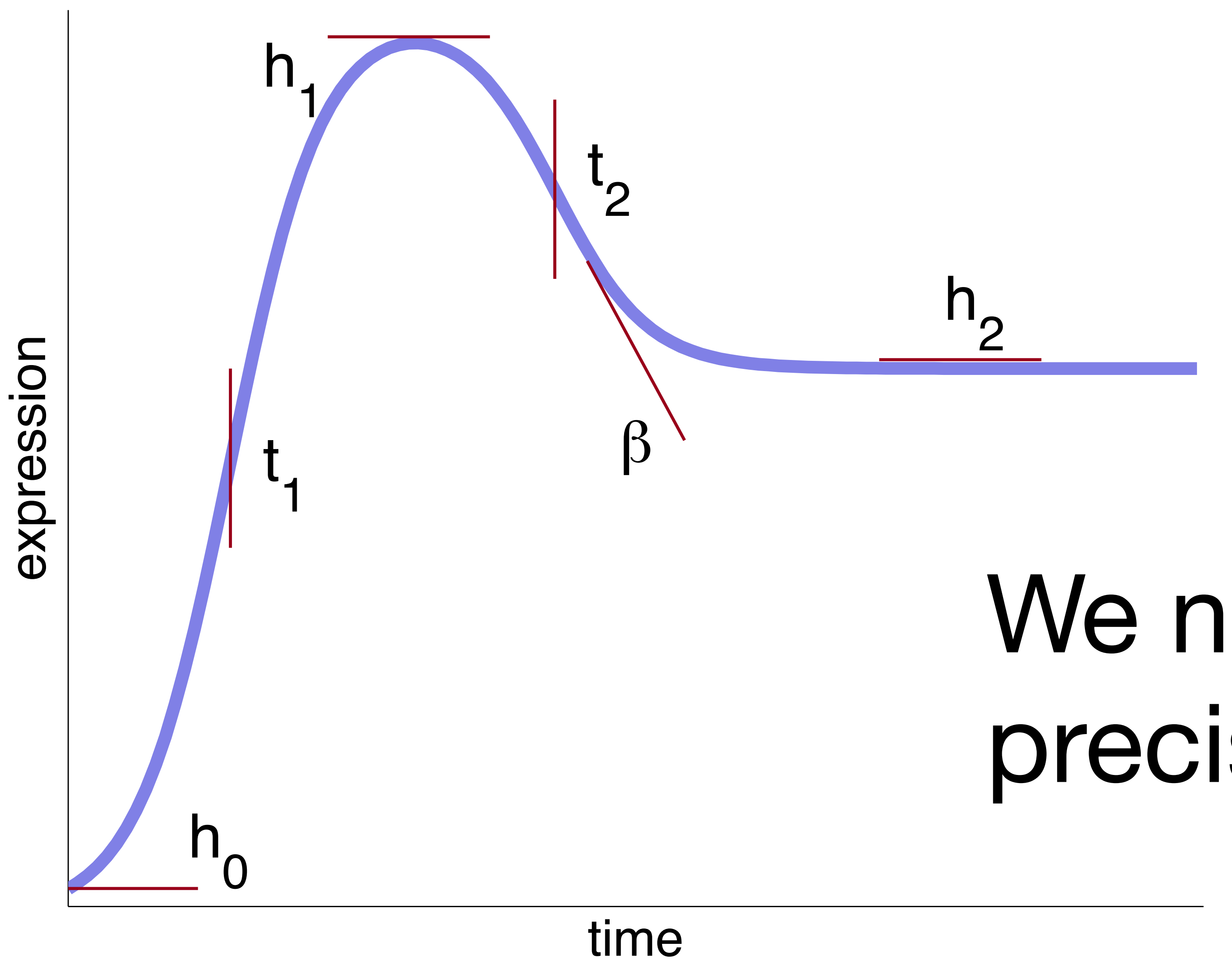
When genomics was data-poor...

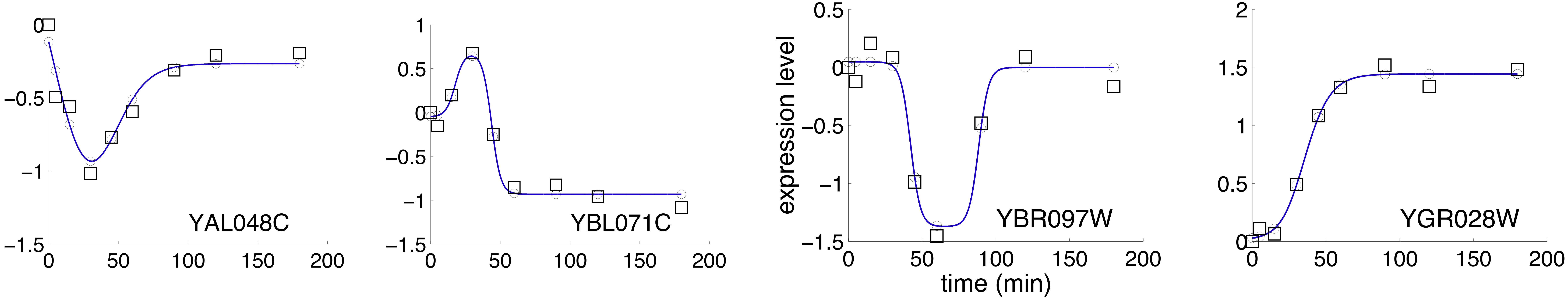
JOURNAL OF COMPUTATIONAL BIOLOGY
Volume 16, Number 2, 2009
© Mary Ann Liebert, Inc.
Pp. 279–290
DOI: 10.1089/cmb.2008.13TT

Timing of Gene Expression Responses to Environmental Changes

GAL CHECHIK and DAPHNE KOLLER

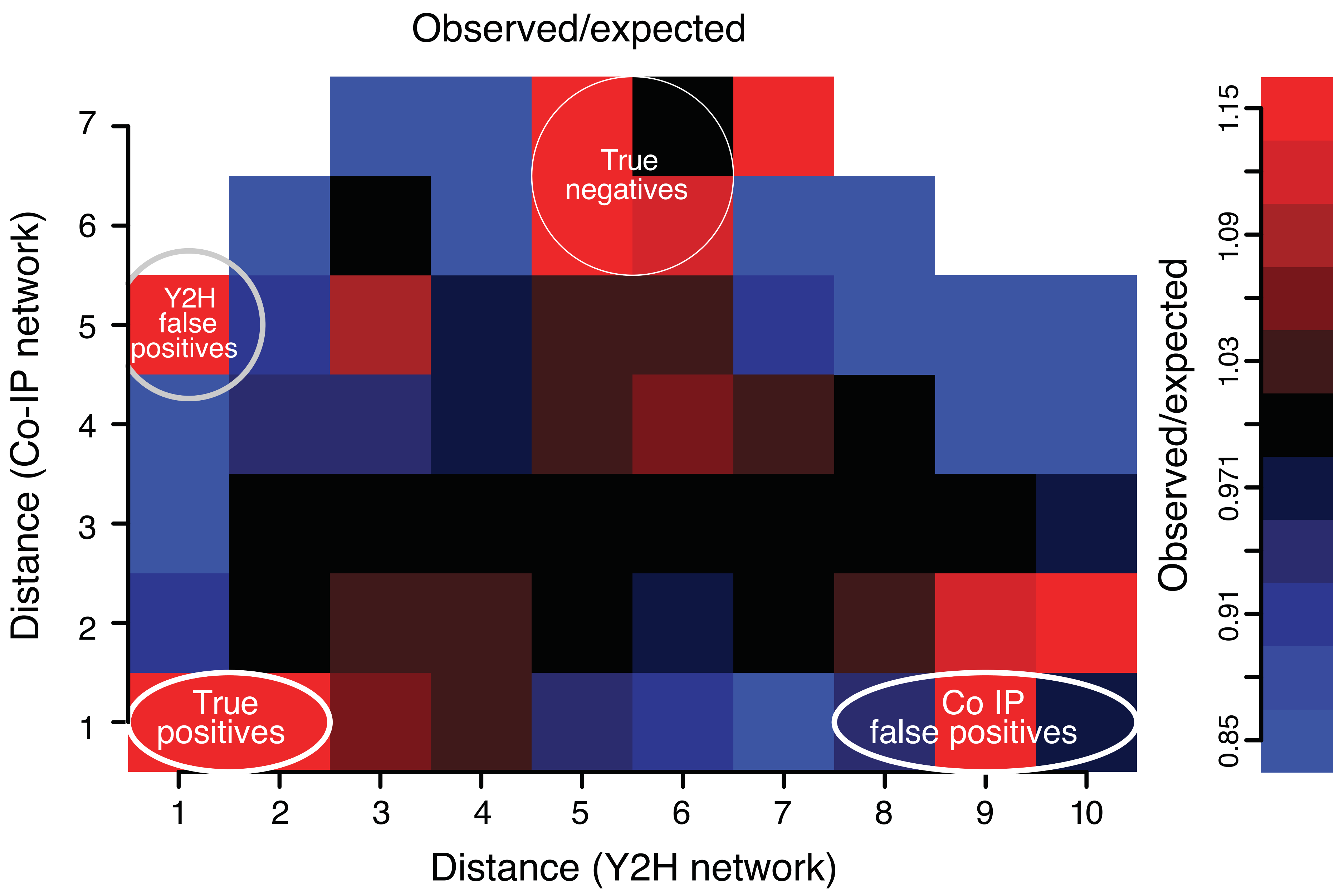


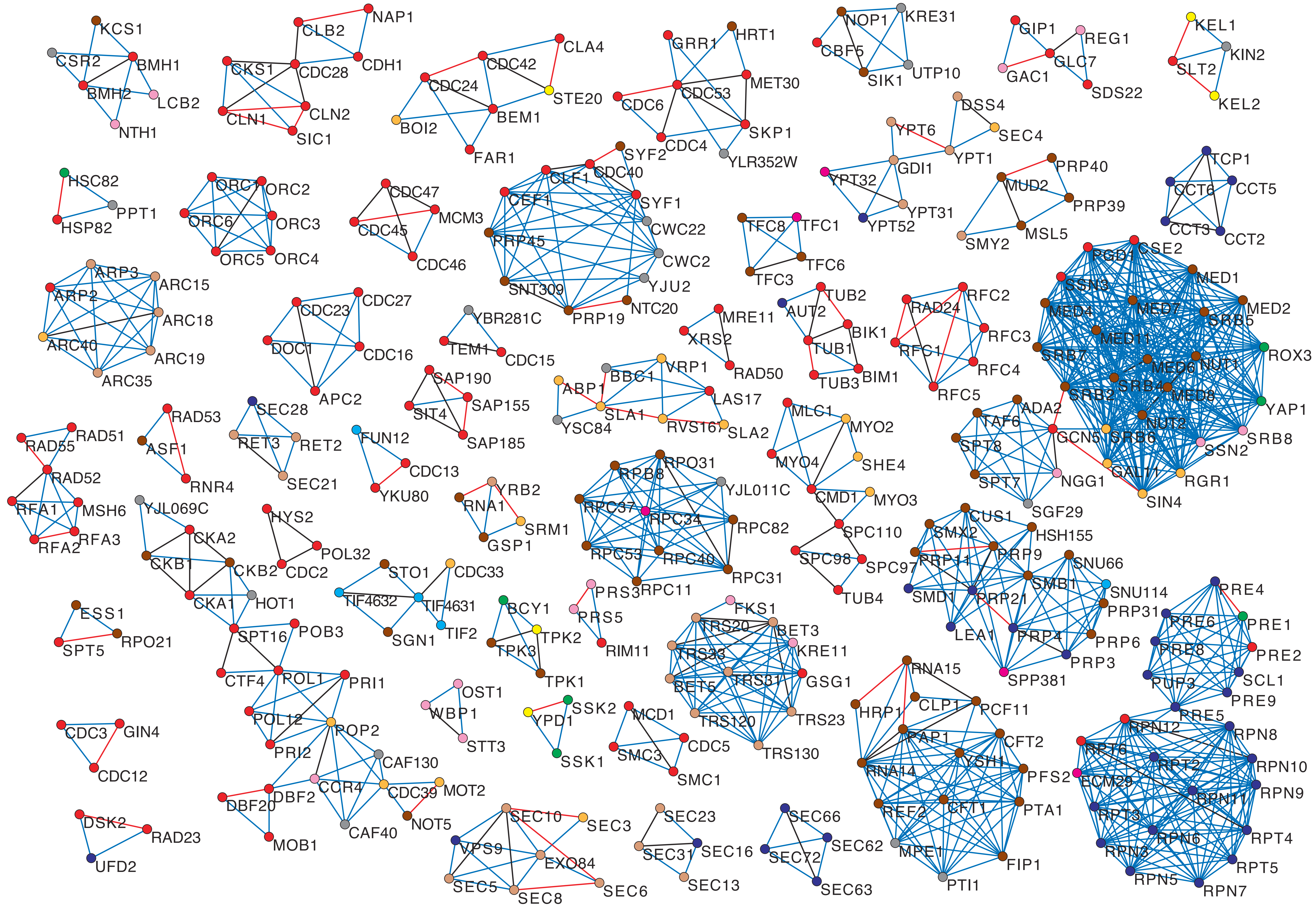
We need a precise model!



Building a just right classification problem was and is still very important.

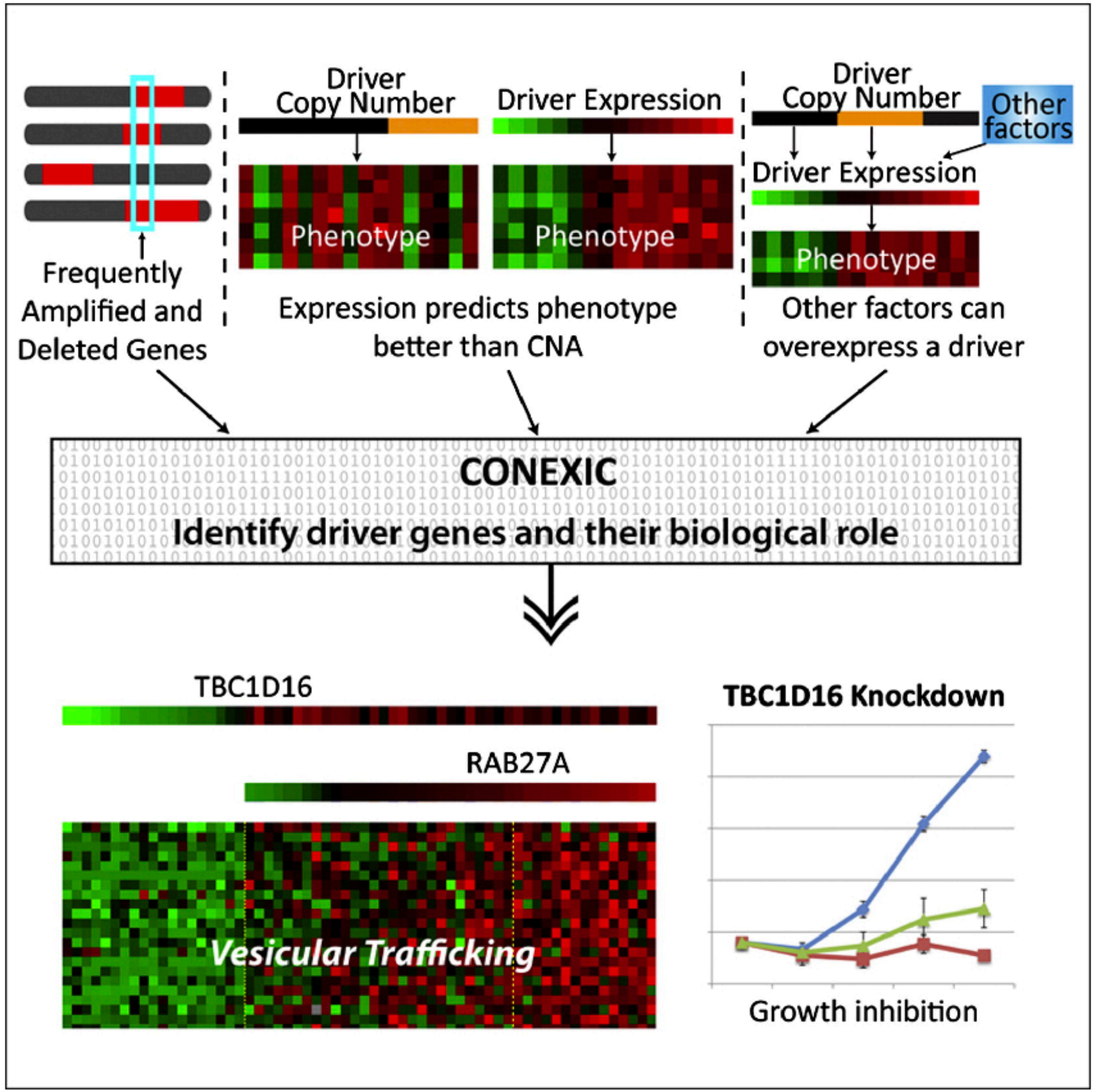
Goal: Can we predict protein-protein interactions?





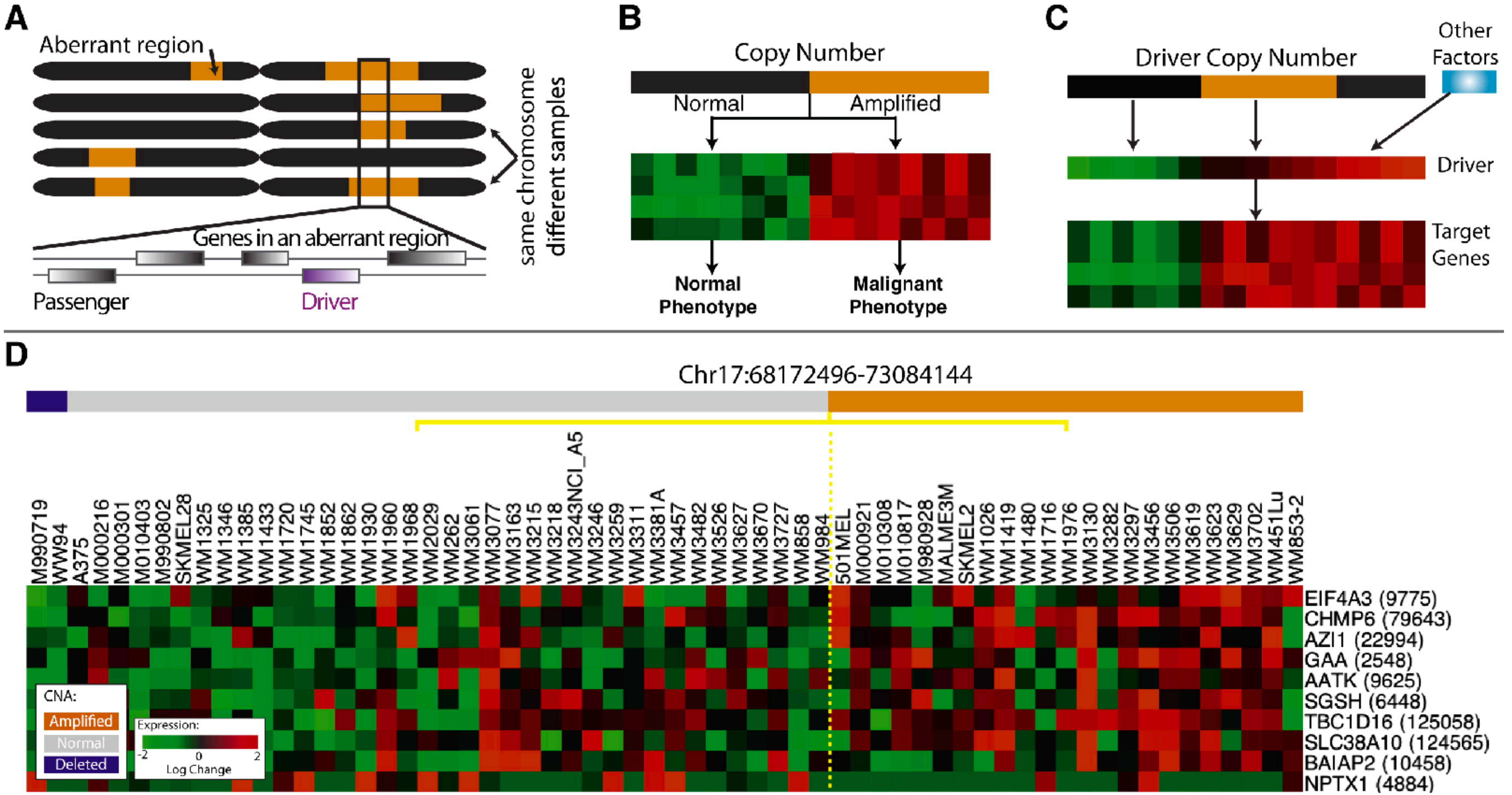
Bader *et al. Nature Biotech* (2004)

Regression is a basic ingredient of linking multiple data modalities



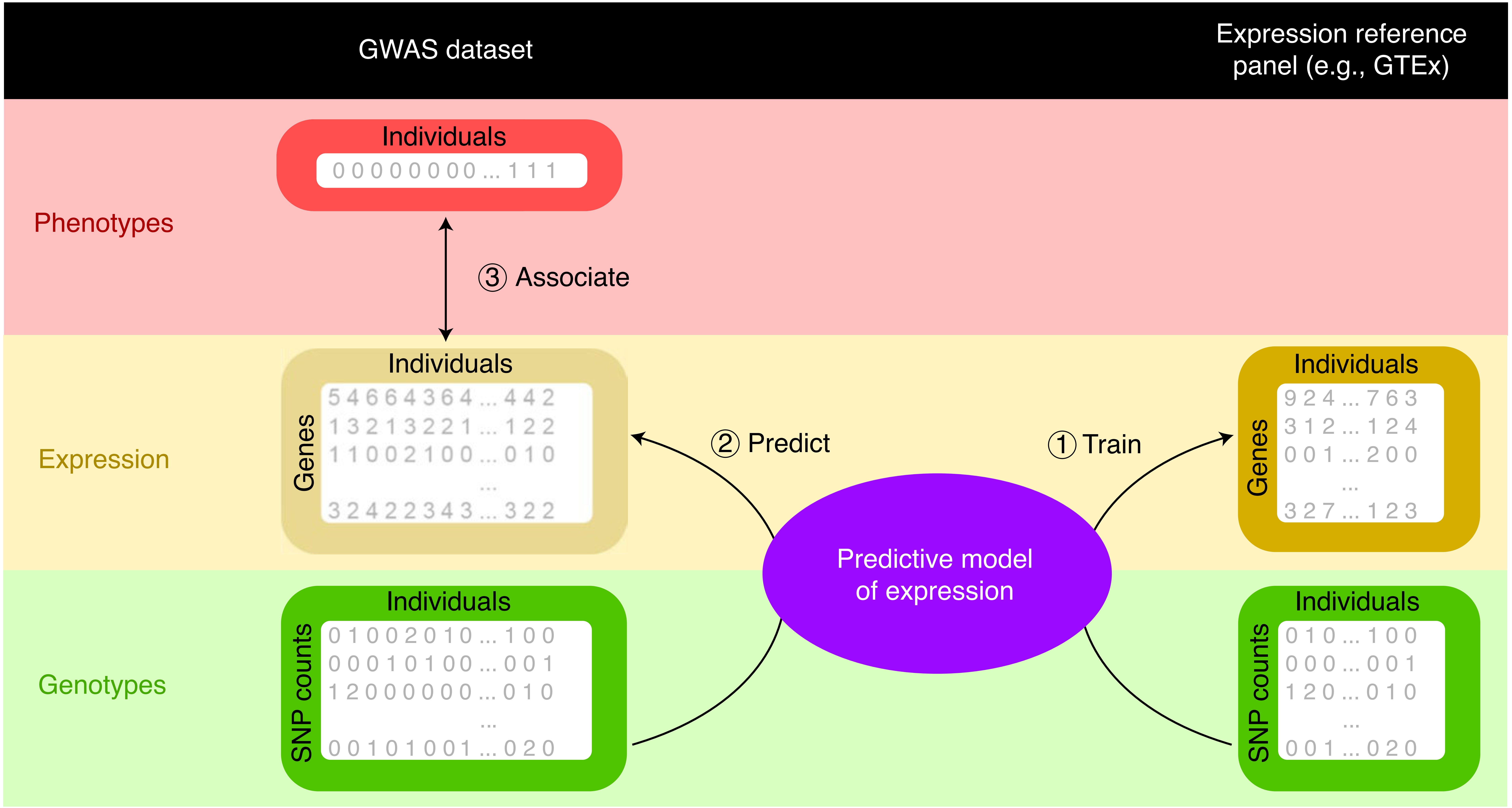
Akavia .. Pe'er, *Cell* (2010)

Regression is a basic ingredient of linking multiple data modalities



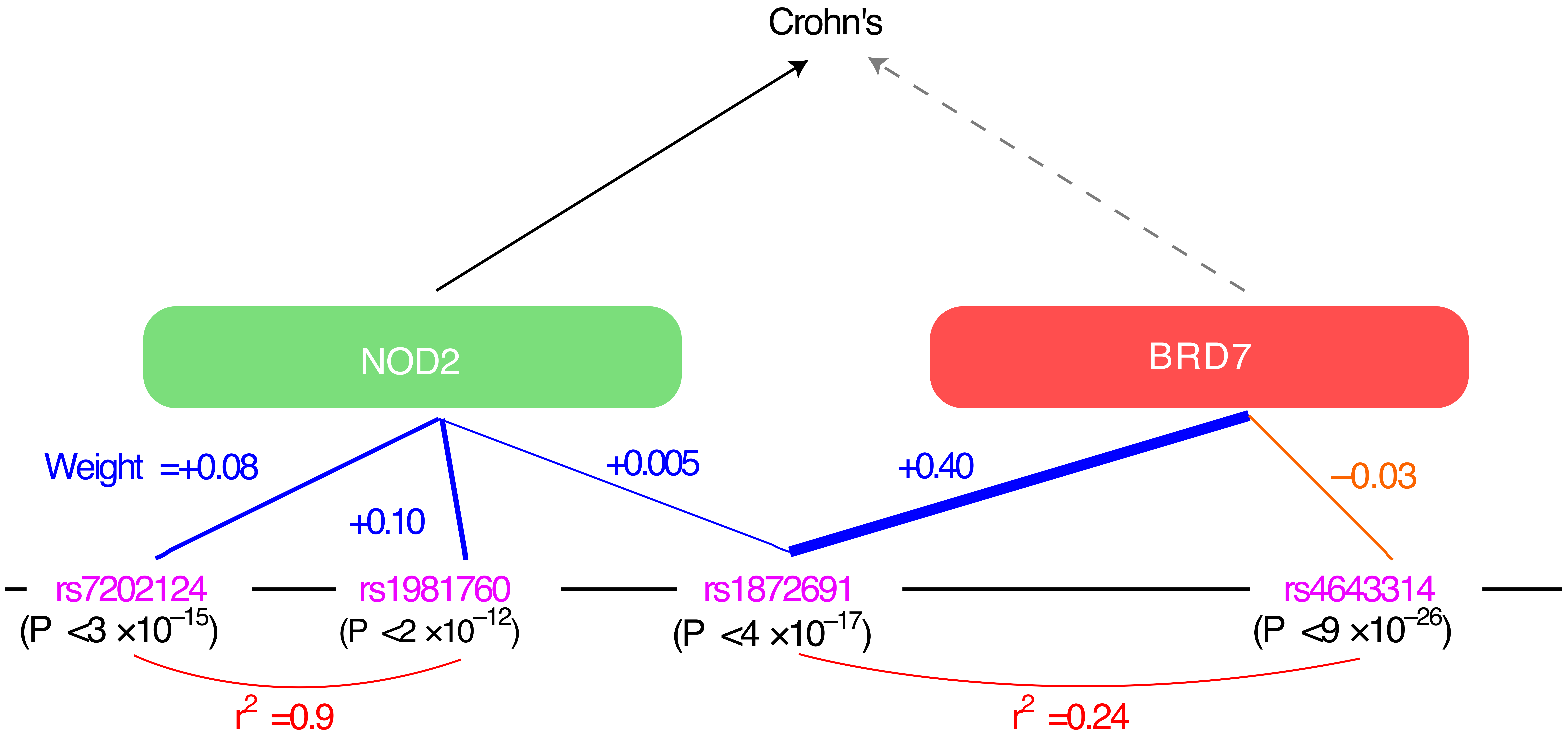
Akavia ..
Pe'er, *Cell*
(2010)

Prediction and association: nuts and bolts of genomics analysis



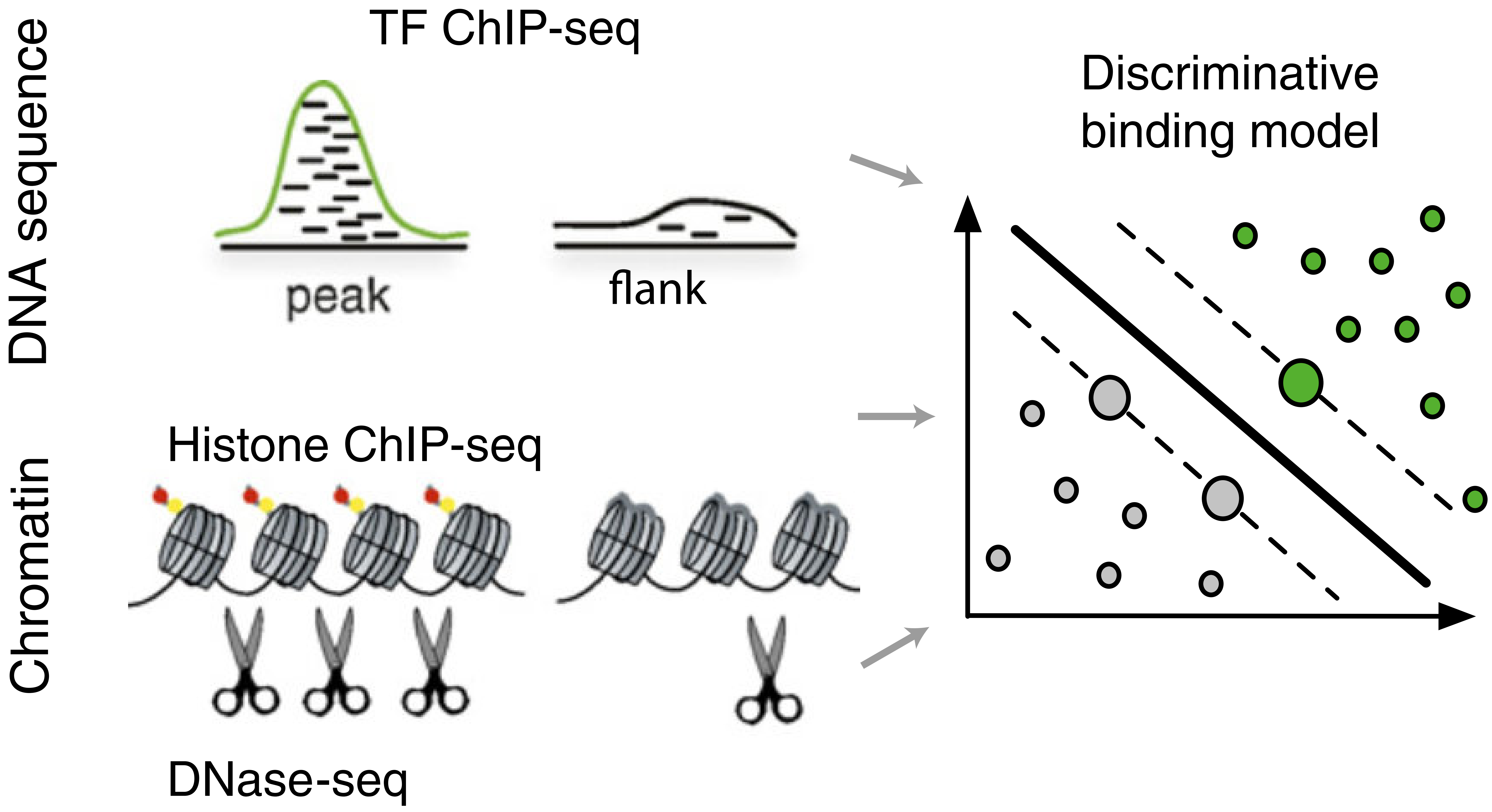
Wainberg .. Im, Pasaniuc, Rivas, Kundaje, *Nature Genetics* (2019)

Prediction of gene expression by genetics followed by associations with disease



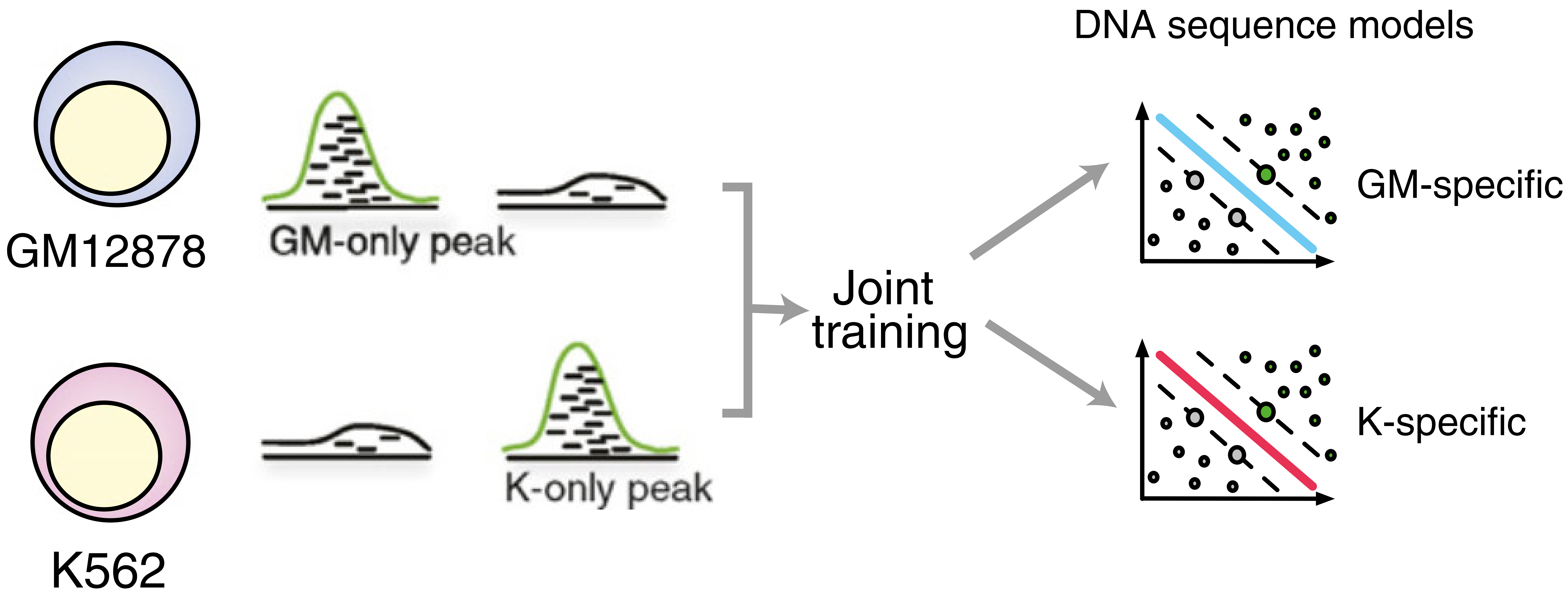
Wainberg .. Im, Pasaniuc, Rivas, Kundaje, *Nature Genetics* (2019)

Why ML in genomics? Augmentation of experimental data



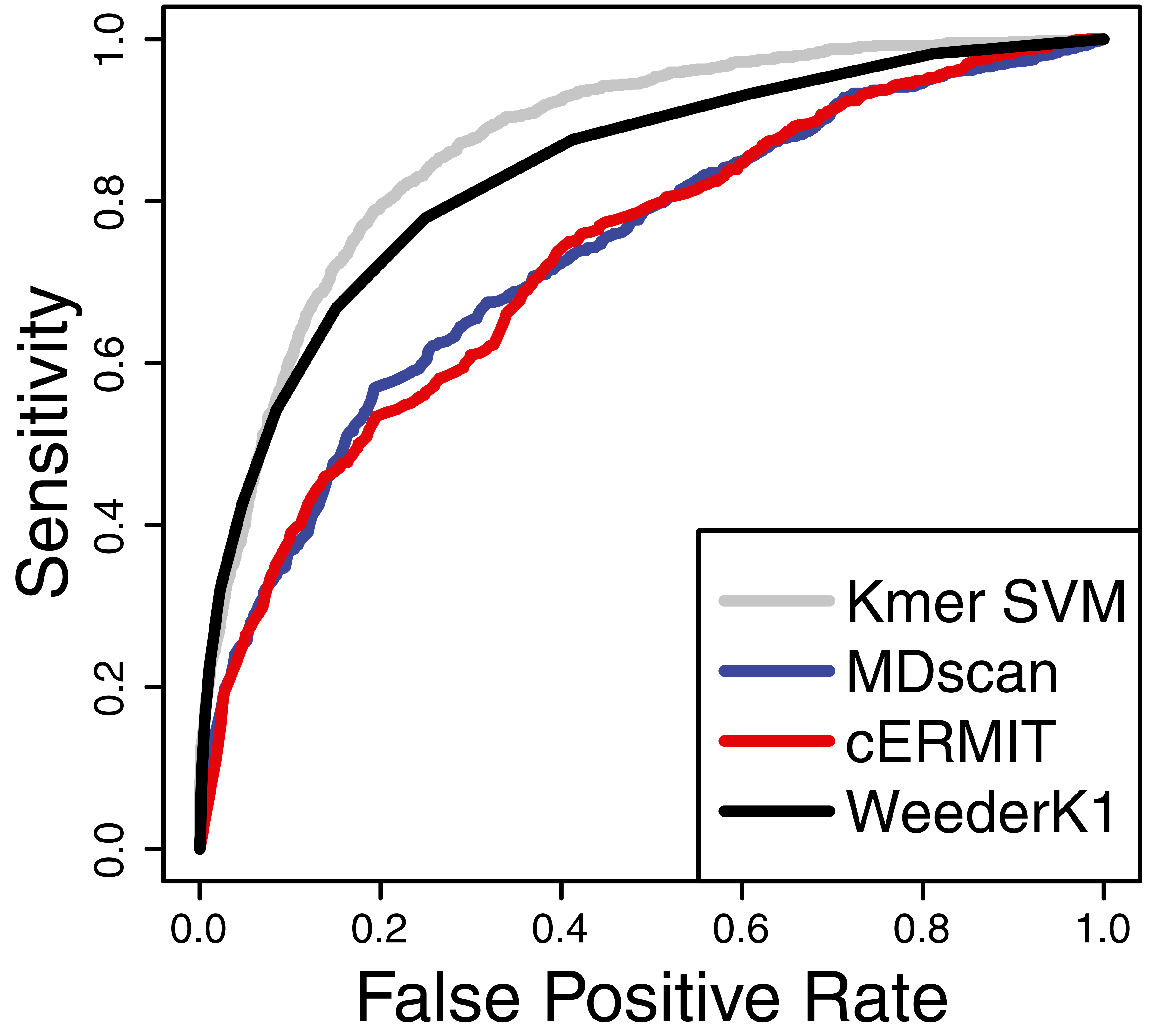
Arvey *et al. Genome Research* (2012)

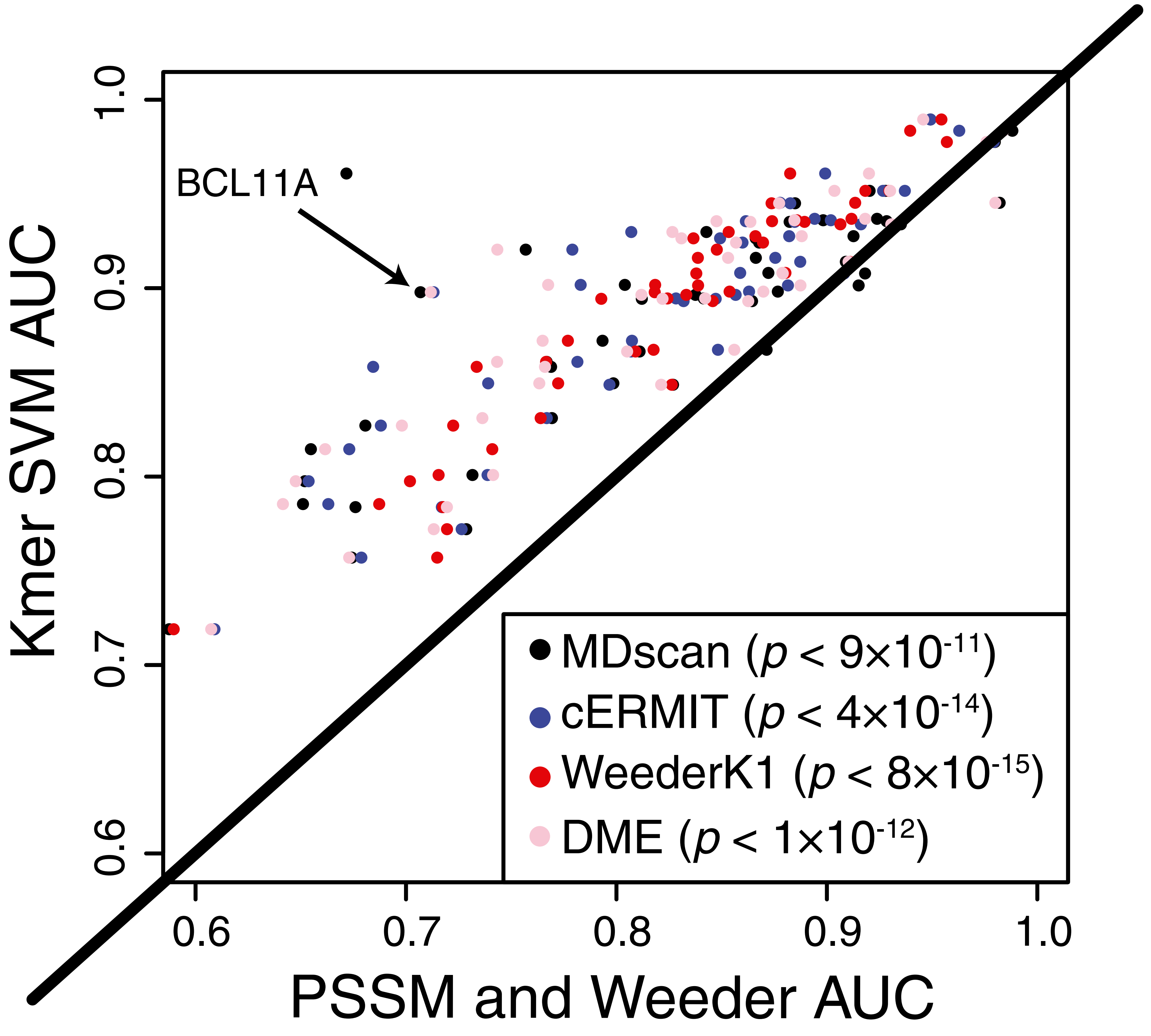
Why ML in genomics? Augmentation of experimental data



Arvey *et al. Genome Research* (2012)

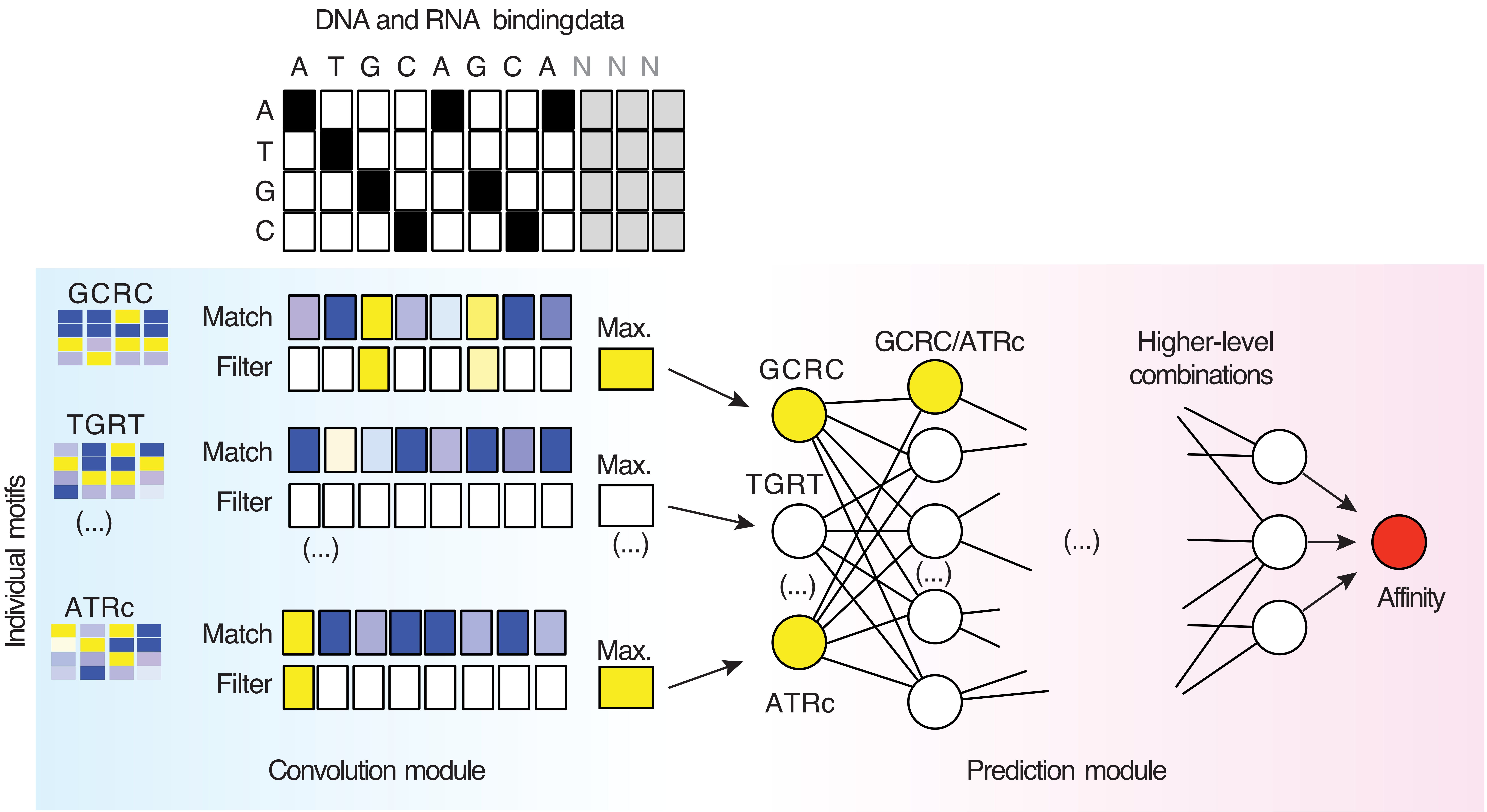
Why ML? ML methods outperform.





Arvey *et al. Genome Research* (2012)

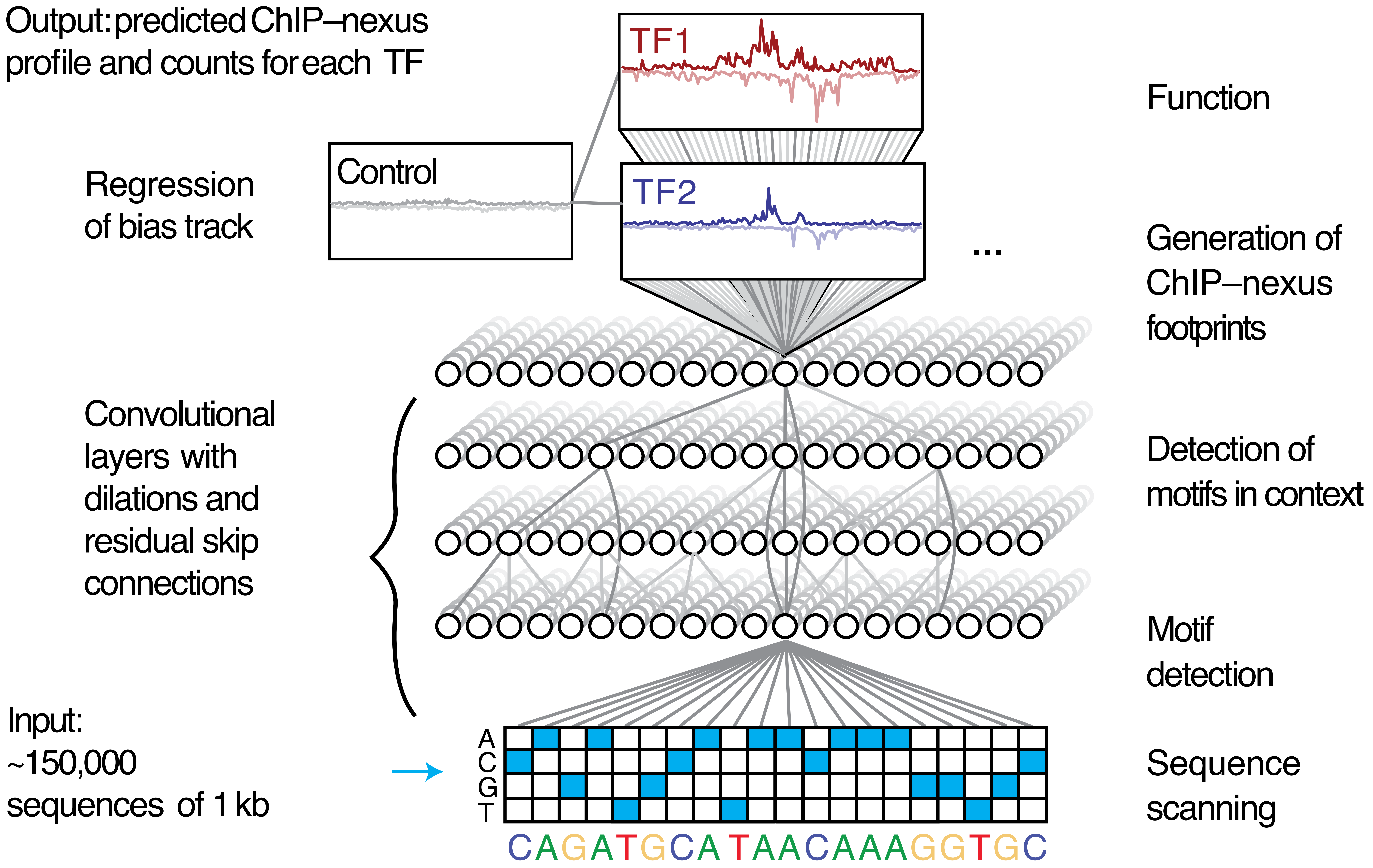
Supervised ML can dissect regulatory elements



Park & Kellis (2015)

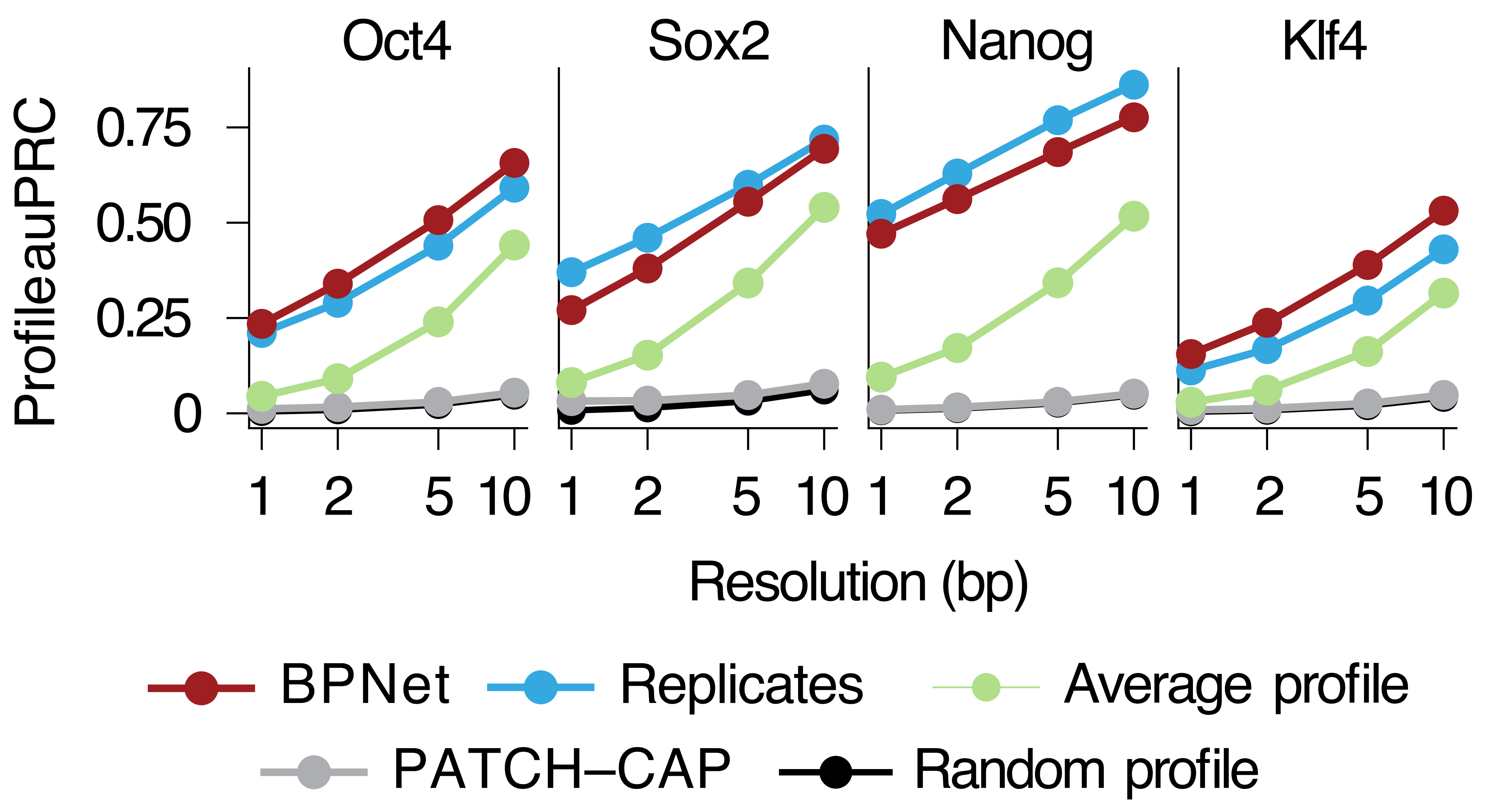
Supervised ML can dissect regulatory elements

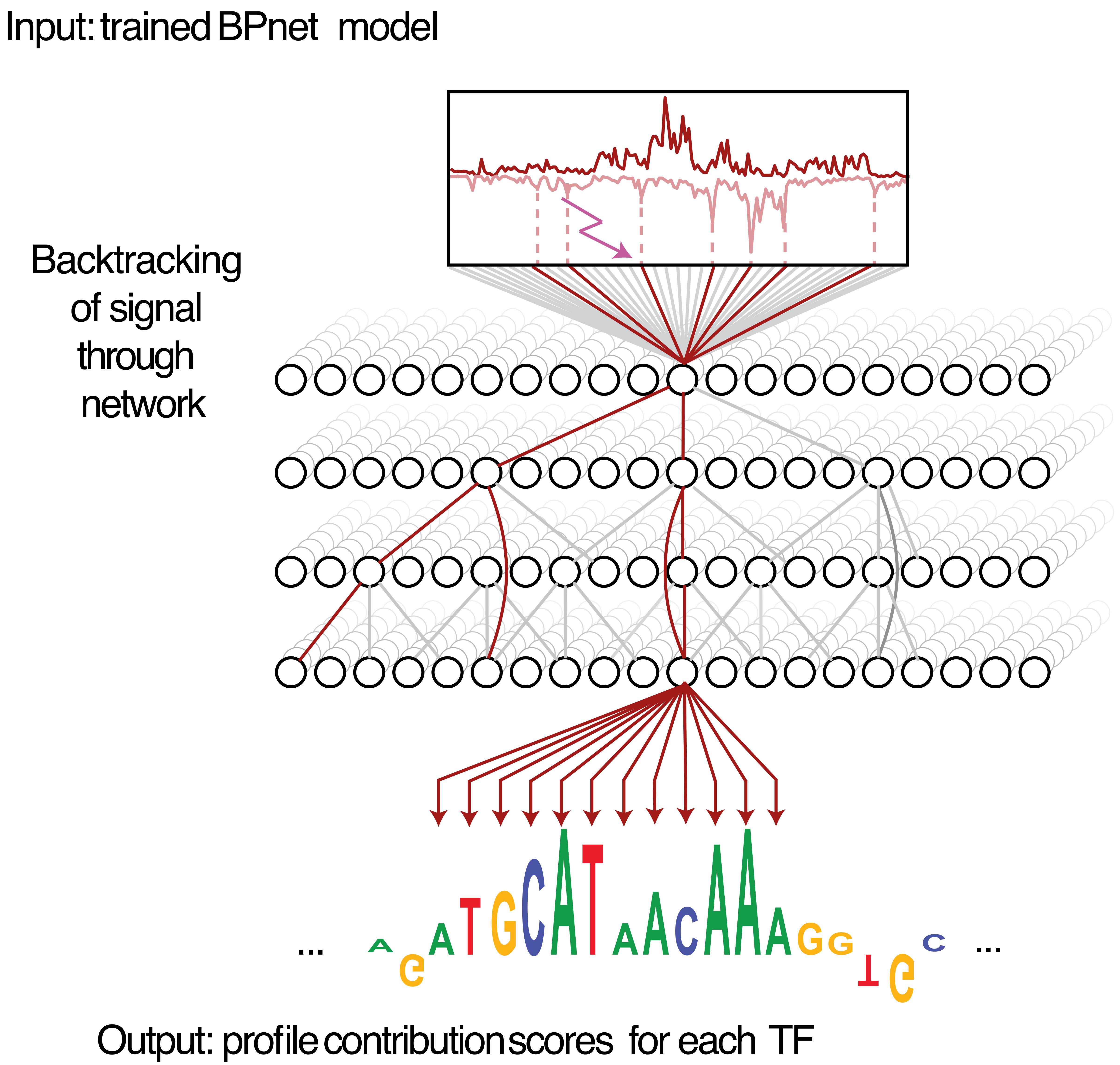
BPNet architecture



Avsec .. Kundaje, Zeitlinger, *Nature Genetics* (2021)

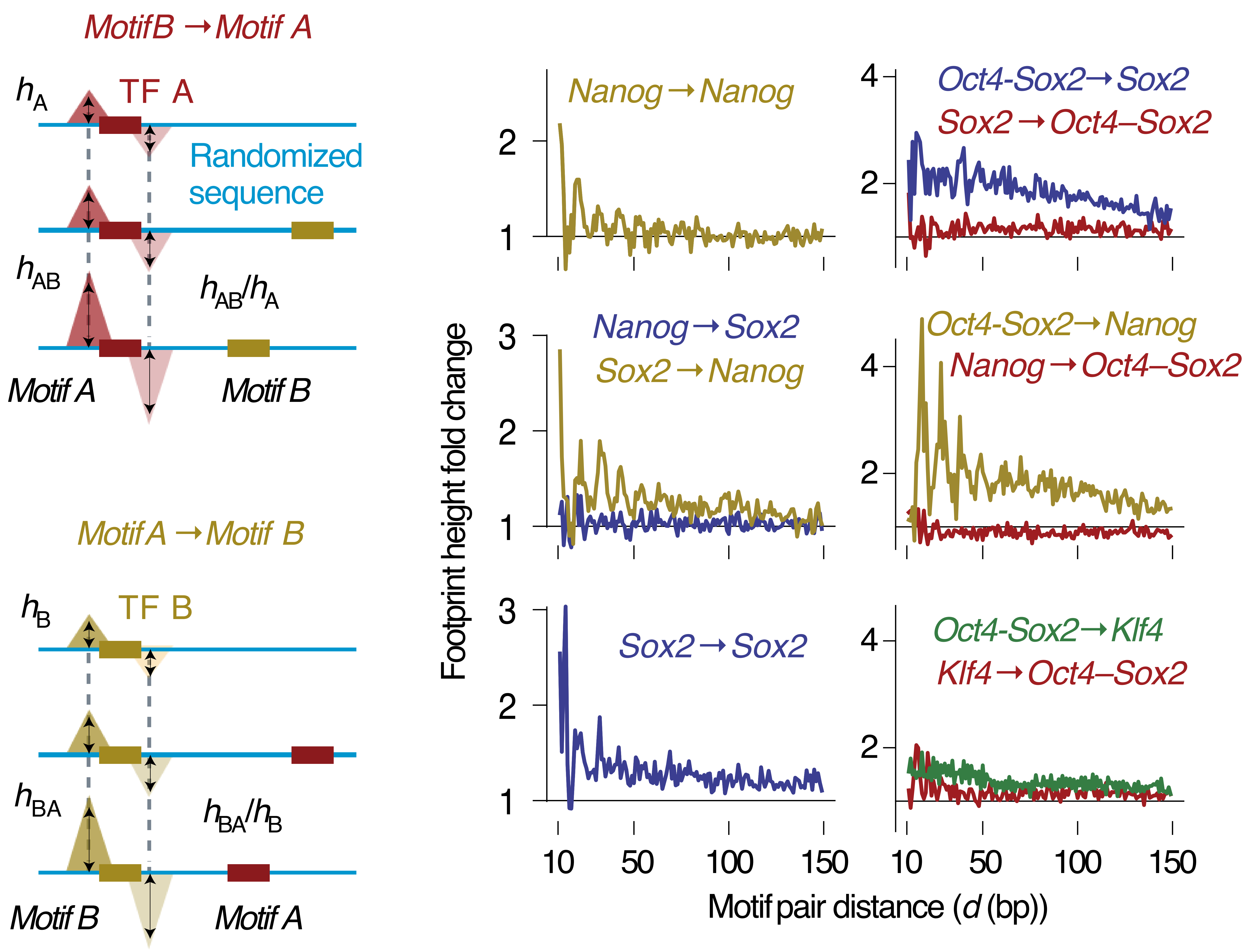
Supervised ML can help understand the logic of biological mechanisms





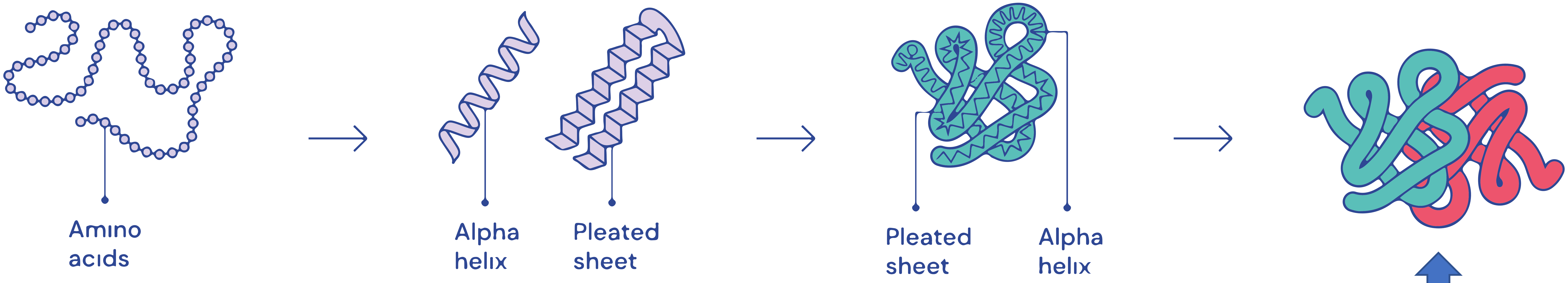
Avsec .. Kundaje, Zeitlinger, *Nature Genetics* (2021)

Accurate prediction, synthetic experiments!



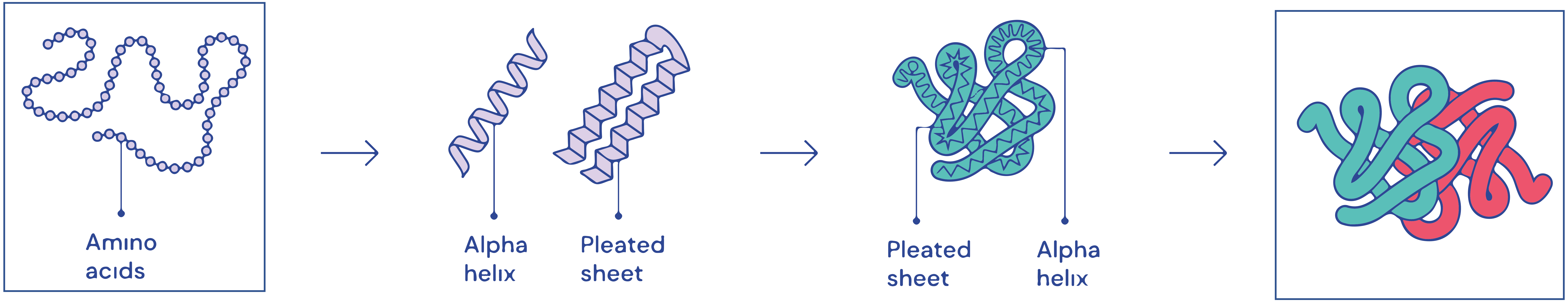
Avsec .. Kundaje, Zeitlinger,
Nature Genetics (2021)

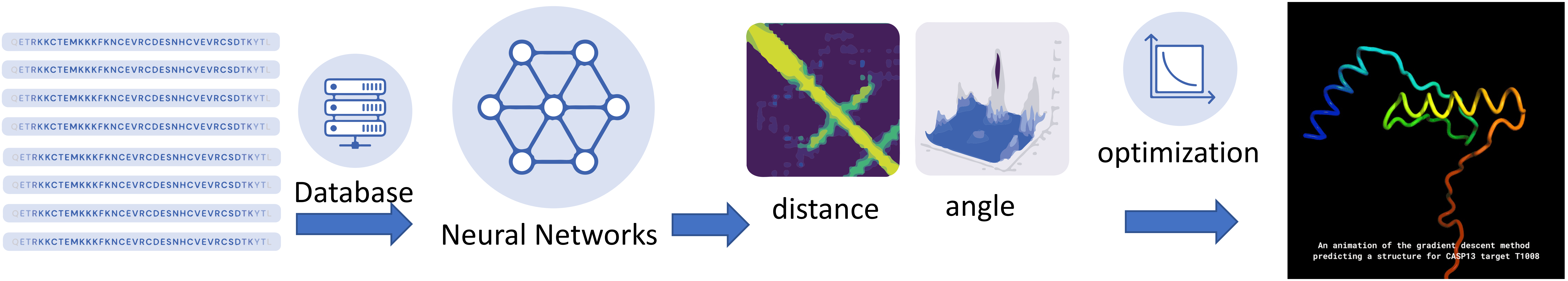
Finally neural networks can predict amino acid (1D) → protein structure (3D)



https://deepmind.com/blog/article/AlphaFold-Using-AI-for-scientific-discovery

Finally neural networks can predict amino acid (1D) → protein structure (3D)





https://deepmind.com/blog/article/AlphaFold-Using-AI-for-scientific-discovery

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What is Supervised Learning?

Supervised learning (today and next lecture)

- Input: data $\mathcal{X} = \{\mathbf{x}_i, ...\}$
- Input 2: label $\mathcal{Y} = \{y_i, ...\}$
- Goal: learn $f : \mathcal{X} \to \mathcal{Y}$

X: gene expression samples; Y: disease labels

Unsupervised learning (previous)

- Input: data $\mathcal{X} = \{\mathbf{x}_i, ...\}$
- Goal 1: learn $f : \mathcal{Z} \to \mathcal{X}$
- Goal 2: hidden/latent states, $\mathcal{Z} = \{\mathbf{z}_i, ...\}$

X: gene expression matrices

Machine learning vs. Classical statistics

Machine Learning

- *"Statistical learning with the help of algorithm"*
- Large number of variables (less scrutiny in variable selection)
- Higher model complexity, non-linearity
- Focusing on **classification/prediction** (that's it)
- Scalability, computation

Classical Statistics

- A handful of variables with clear idea
- A (generalized) linear model
- Data generating process (Bayesian)
- More focuses on **scrutiny** (type-I-error, FDR, etc) and **variable selection**

Note: We take a bit more statistical stance.

Four Steps for Supervised Learning

1. Gather some training data (this is a part of research!):

$$\begin{aligned} \mathcal{X} &\equiv \{\mathbf{x}_i : i \in [n]\} && \text{predictors/covariates/features} \\ \mathcal{Y} &\equiv \{\mathbf{y}_i : i \in [n]\} && \text{outcome/response} \end{aligned}$$

2. Write down a model (classifier) $f : \mathcal{X} \to \mathcal{Y}$
   - What is the loss function?
3. Fit the model to the training data
4. Use the model
   - We can focus on the interpretation of model parameters
   - We can focus on prediction on *new* data points

Today's lecture

General discussions on supervised learning

Classification with a decision rule

Generalized linear model

Generative Modelling approach

Other Methods

Both regression and classification is supervised

Multivariate Linear Regression

- X: $n \times p$ design matrix
- $\mathbf{y}$: $n \times 1$ outcome vector
- β_k: a regression coefficient for a covariate k
- ϵ: a vector of residual errors
- A regression model:

$$Y_i = \sum_k X_{ik}\beta_k + \epsilon_i$$

(or $\mathbf{y} = X\beta + \epsilon$)

Both regression and classification is supervised

Multivariate Linear Regression

- X: $n \times p$ design matrix
- $\mathbf{y}$: $n \times 1$ outcome vector
- β_k: a regression coefficient for a covariate k
- ϵ: a vector of residual errors
- A regression model:

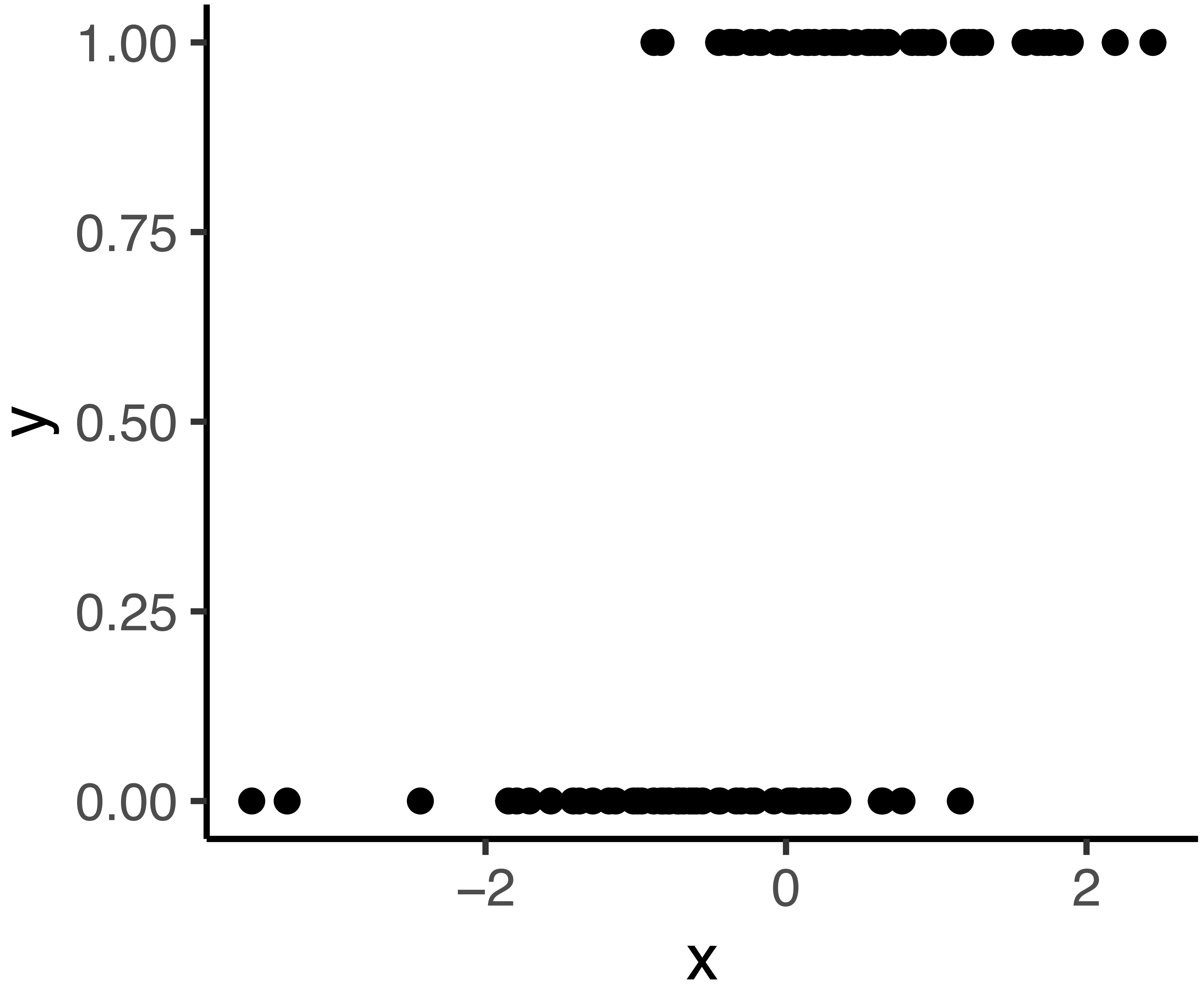
$$\mathbf{y} = X\beta + \epsilon$$

(A linear) Classifier

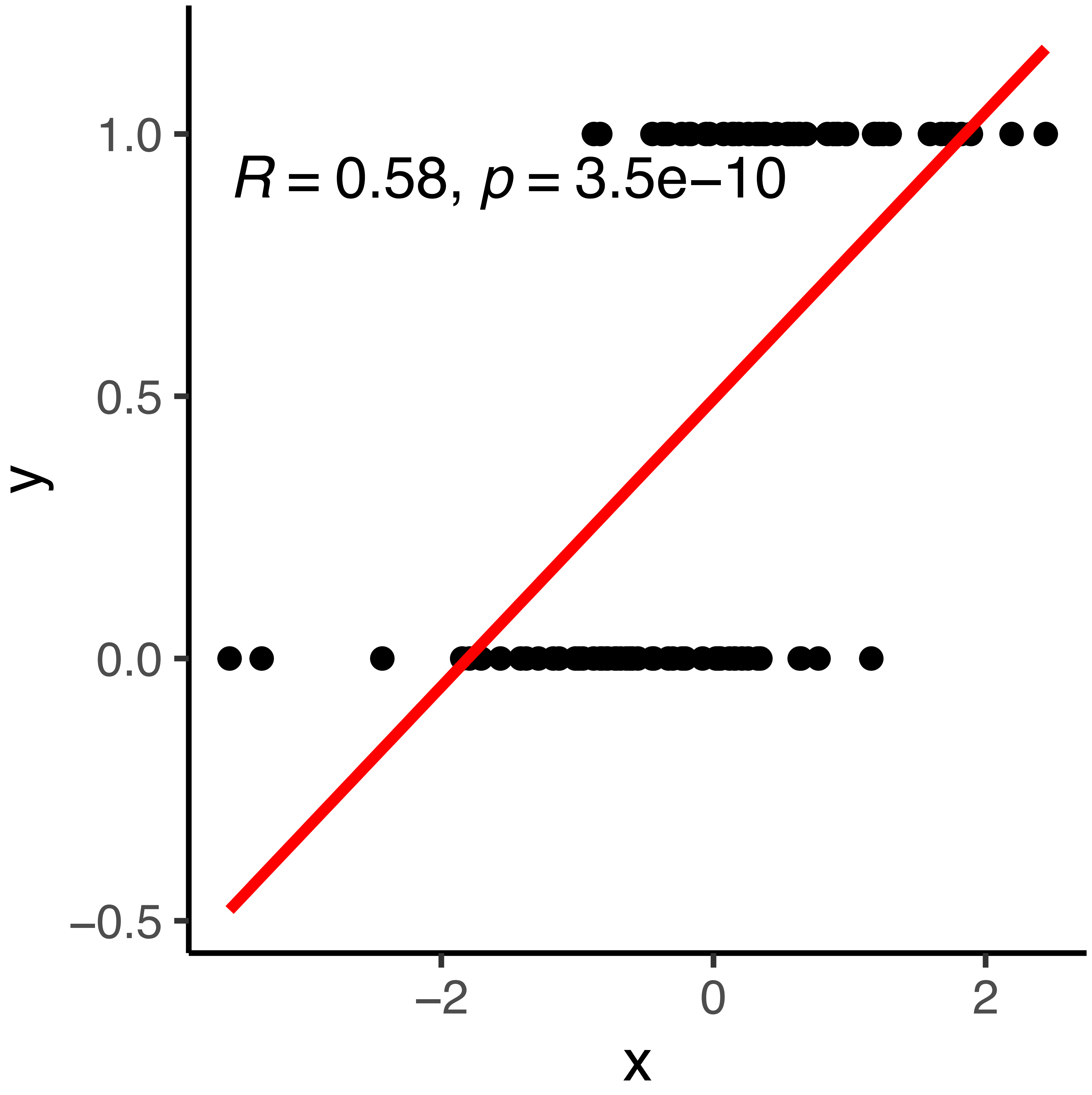
- X: $n \times p$ design matrix
- $\mathbf{y}$: $n \times 1$ **class label** vector, e.g., $\{0, 1\}^n$
- β_k: a coefficient for a covariate k
- A prediction model:

$$Y_i \leftarrow f\left(\sum_k X_{ik}\beta_k\right)$$

A primer question: Can we simply use regression for classification?



A primer question: Can we simply use regression for classification?



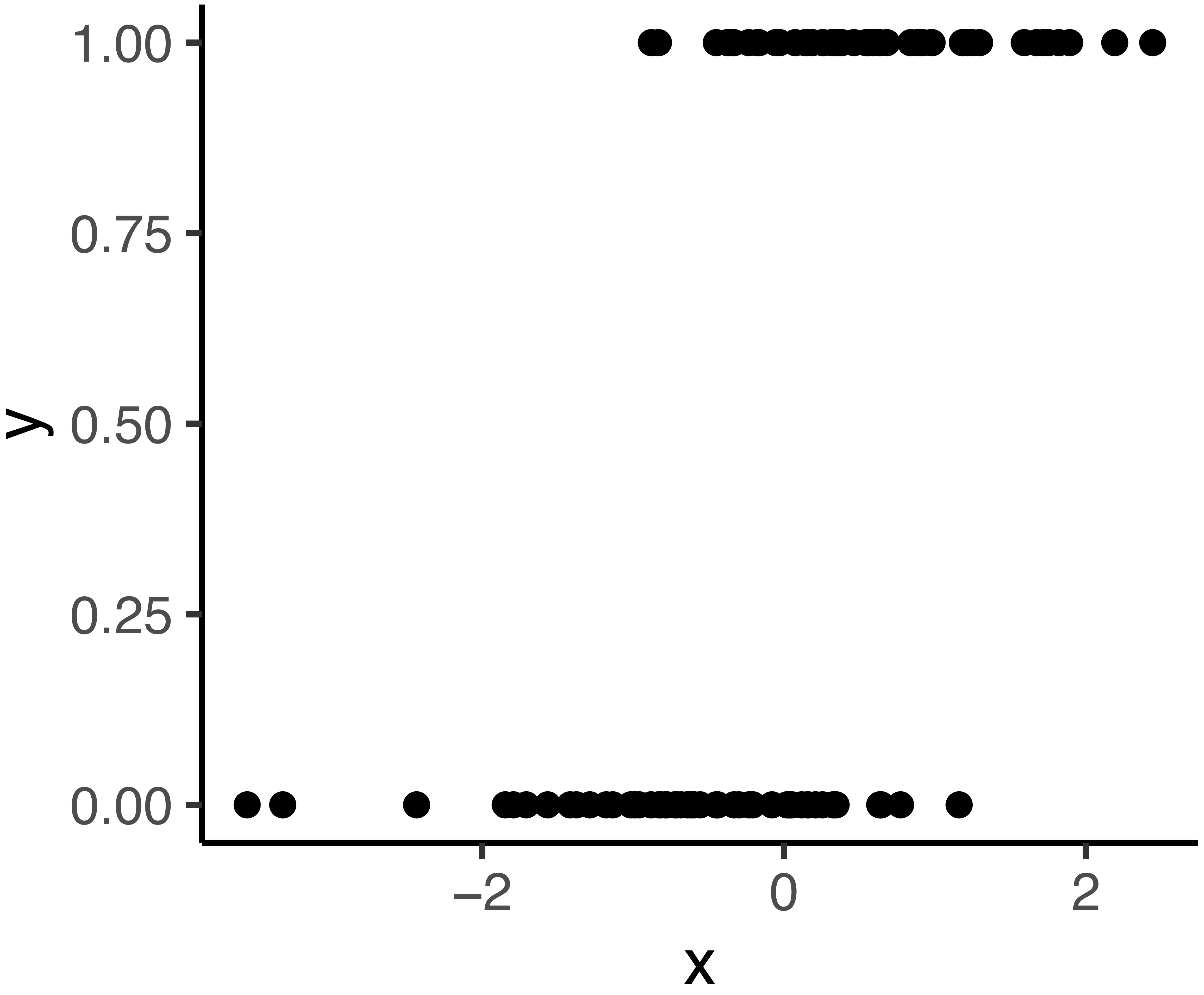
We don't need to cover all the "areas" of Y

```r
.glm <- glm(y ~ x, family="binomial")
```

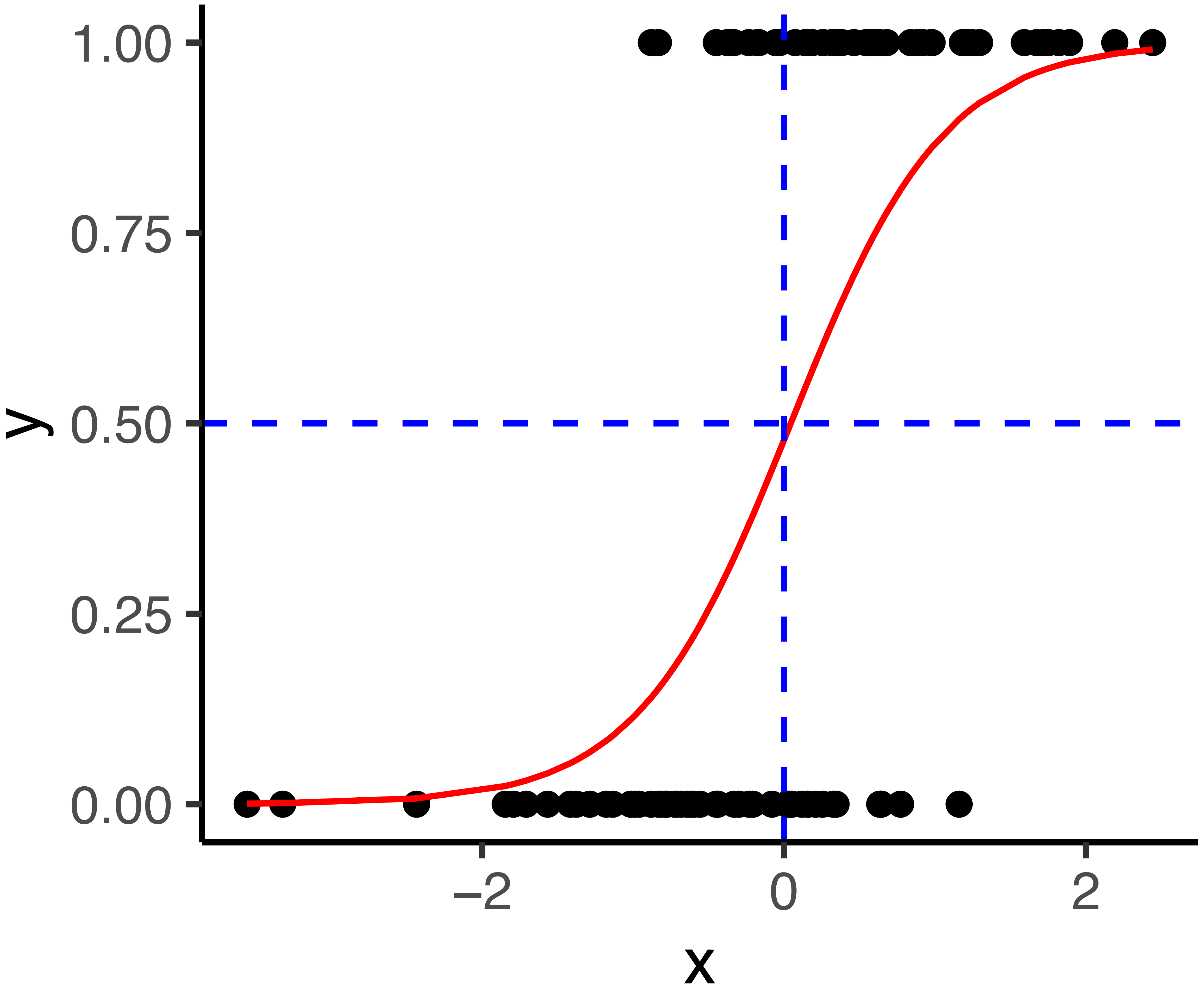
Unlike $X_i \in \mathbb{R}$, we have

$$Y_i \in \{0, 1\}$$

Classification = drawing a decision boundary

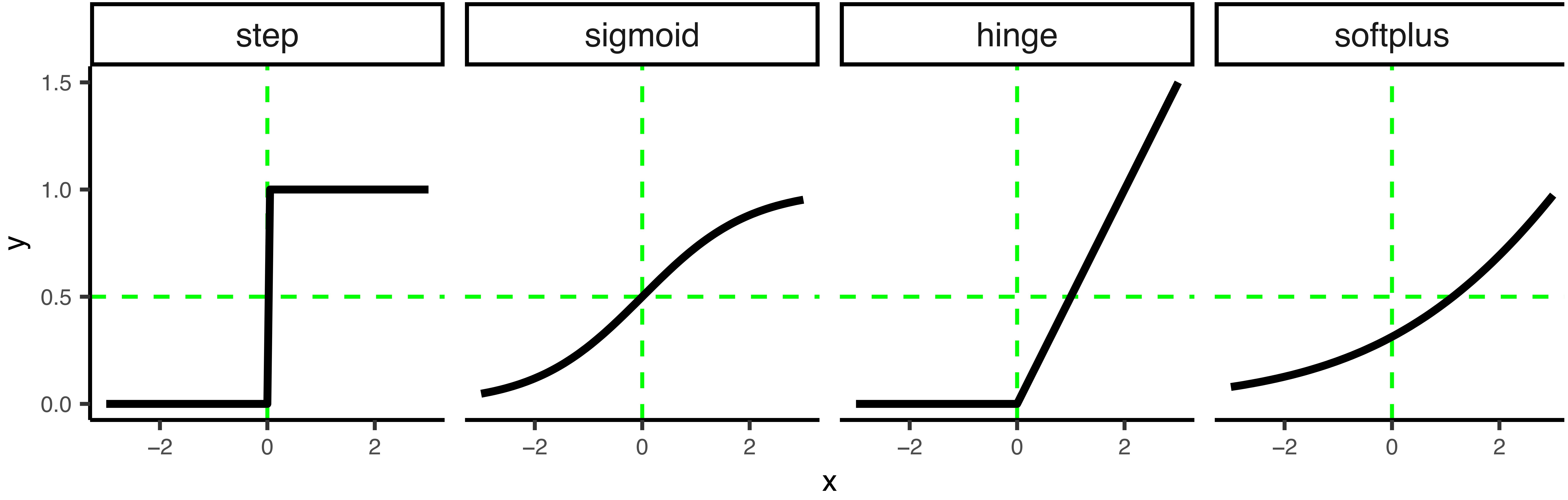


Classification = drawing a decision boundary



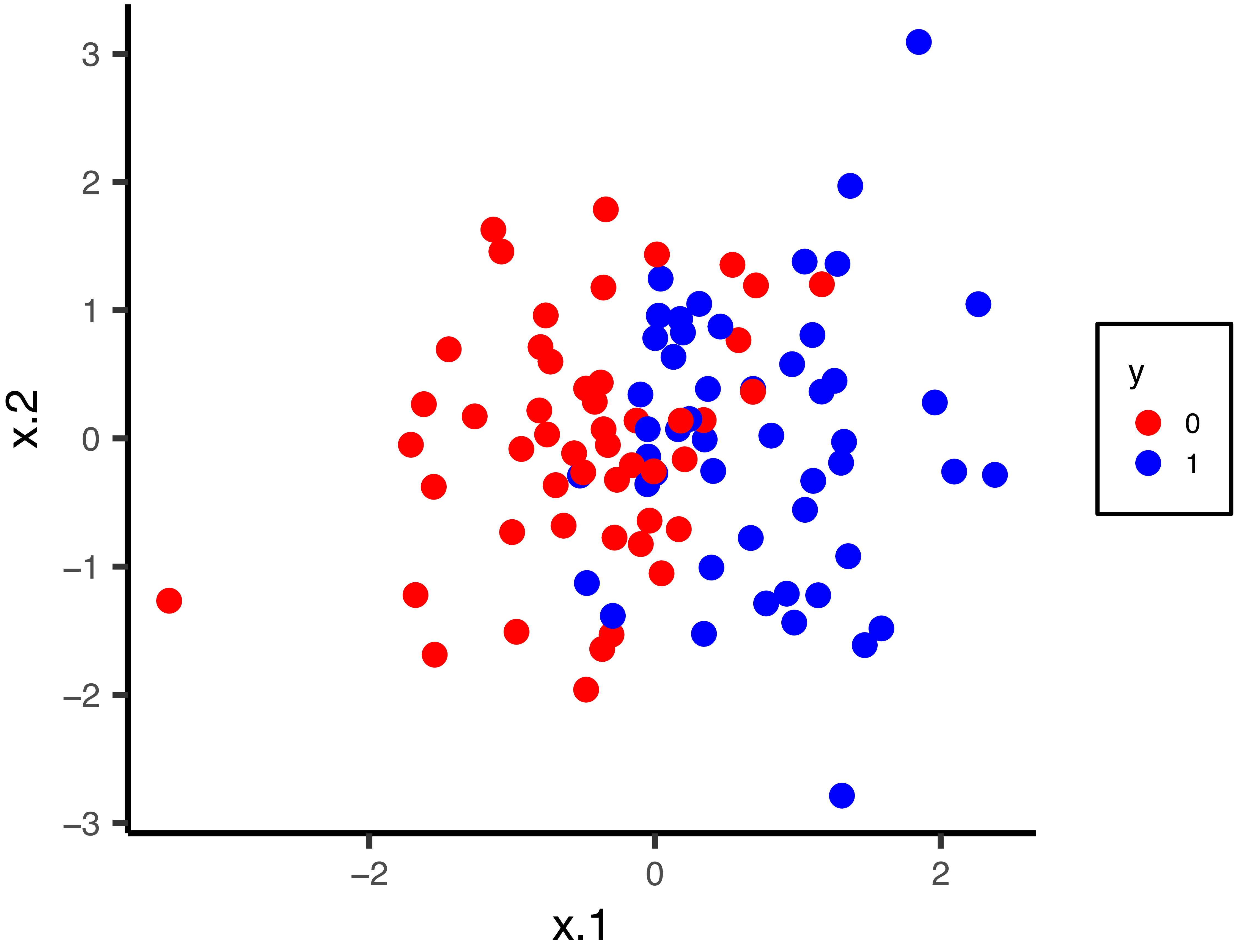
Step-like functions

We will use a step-like function to approximate classification rules



$$f(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases},\ f(x) = \frac{e^x}{1+e^x},\ f(x) = \max\{0, x\xi\},\ f(x) = \log(1+\exp(x\alpha - \beta))$$

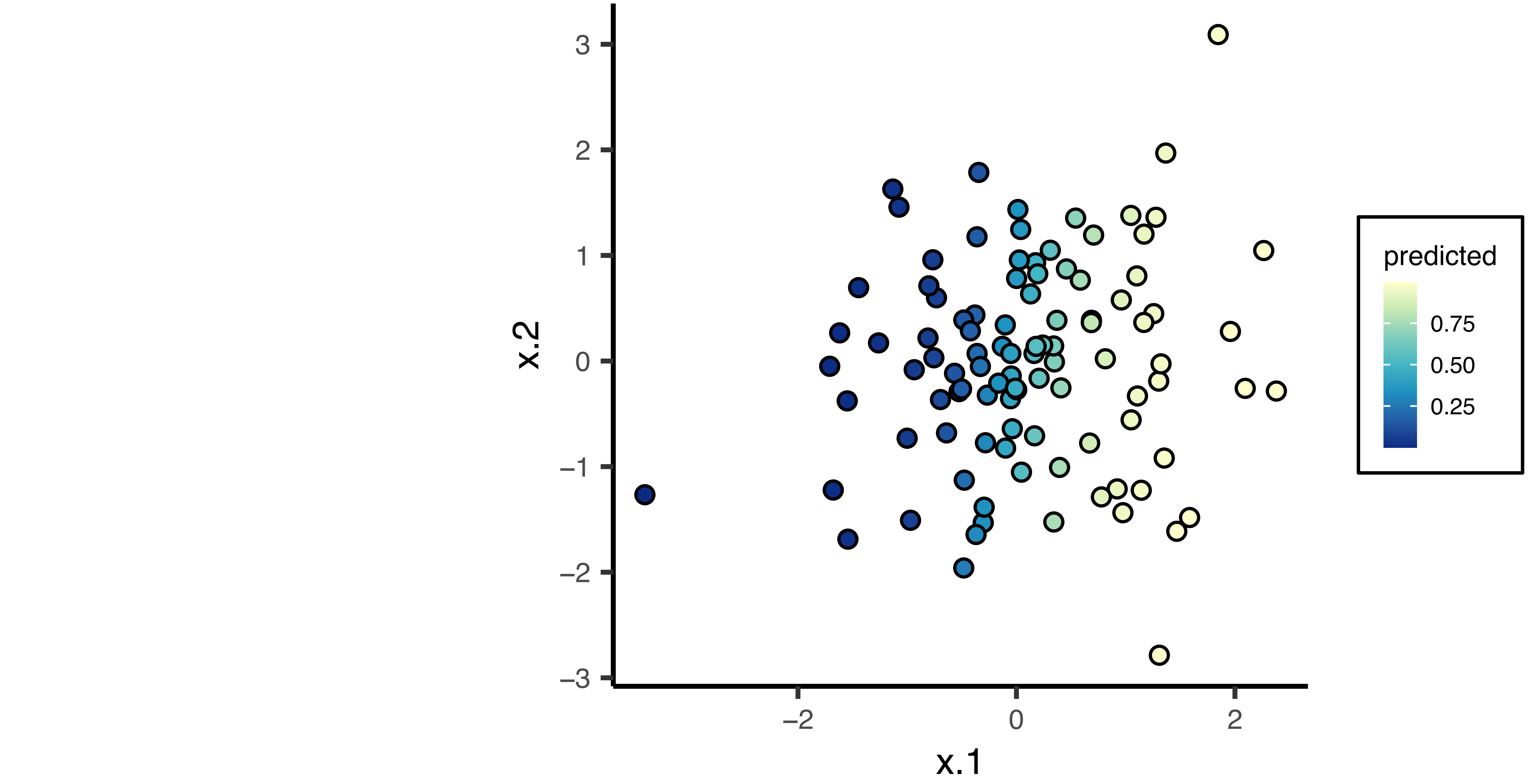
Classification = drawing a decision boundary - 2D



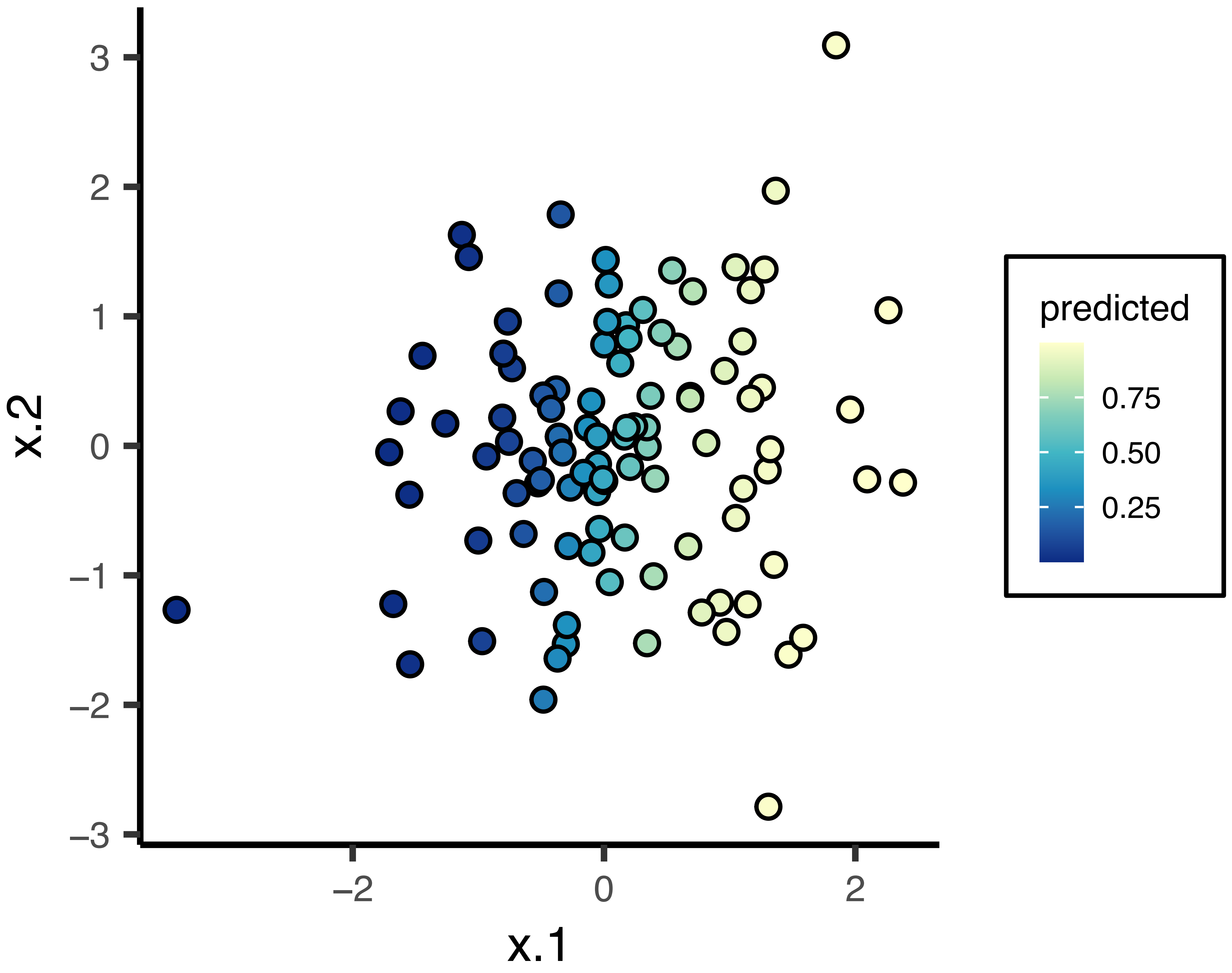
Classification = drawing a decision boundary - 2D

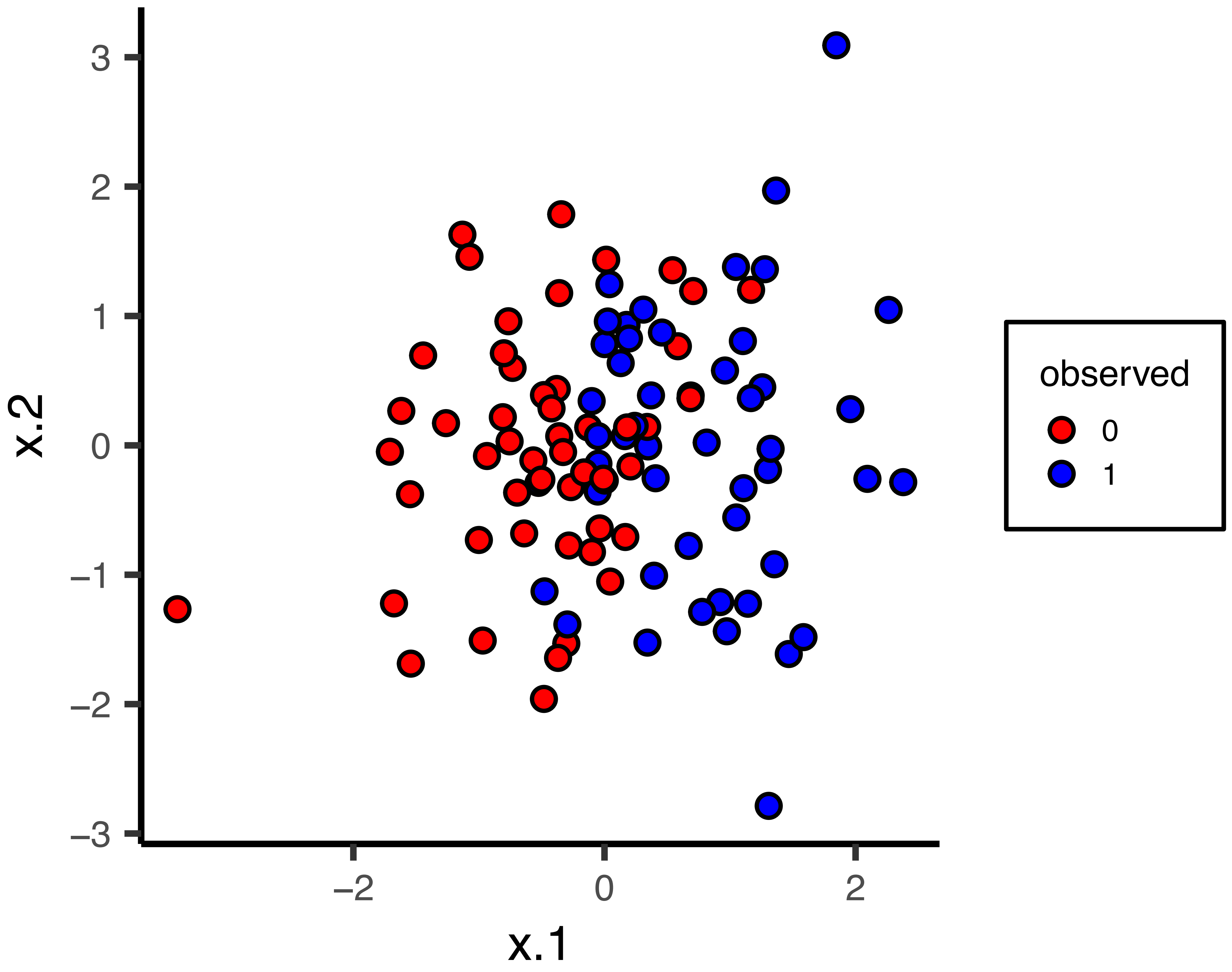
```
.glm <- glm(y ~ x, family = "binomial")
y.hat <-  fitted(.glm)
```

Classification = drawing a decision boundary - 2D



Classification = drawing a decision boundary - 2D





Understanding loss functions (regression vs. classification)

Regression loss

$$L_n = n^{-1} \sum_{i=1}^{n} \big(\underbrace{y_i}_{\text{observed}} - \underbrace{\mathbf{x}_i \beta}_{\text{predicted}} \big)^2$$

Average distance between the observed and predicted.

Classification loss

Given a classifier spits out class label, e.g., $\{0, 1\}$,

$$L_n = n^{-1} \sum_{i=1}^{n} I \left\{ \underbrace{y_i}_{\text{observed}} \neq \underbrace{f\left(\mathbf{x}_i \beta\right)}_{\text{predicted}} \right\}$$

Average frequency of a wrong answer by the classifier.

- **Algorithm:** Minimize the loss function with respect to free parameters β.

Logistic regression: a probabilistic version of classification loss

If a classifier $f(\mathbf{x}_i \beta) \in (0, 1)$ provides a probability of $Y_i = 1$, $\hat{p}(Y_i | \mathbf{x}_i, \beta)$:

Bernoulli likelihood:

$$\prod_{i=1}^{n} f^{Y_i} (1 - f)^{1 - Y_i}$$

Logistic regression: a probabilistic version of classification loss

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Bernoulli likelihood:

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where for each data point i

$$\text{likelihood}_i = \begin{cases} f & \text{if } Y_i = 1 \\ (1-f) & \text{if } Y_i = 0 \end{cases}$$

We will use the sigmoid function

$$f(z) = \frac{e^z}{1+e^z}$$

Logistic regression: a probabilistic version of classification loss

If a classifier $f(\mathbf{x}_i\beta) \in (0,1)$ provides a probability of $Y_i = 1$, $\hat{p}(Y_i|\mathbf{x}_i, \beta)$:

Bernoulli likelihood:

$$\prod_{i=1}^{n} f^{Y_i}(1-f)^{1-Y_i}$$

We can use negative log-likelihood as a "softer" version classification loss

$$L = -\log \sum_{i=1}^{n} \left[f(\mathbf{x}_i\beta)^{Y_i} \left[1 - f(\mathbf{x}_i\beta)\right]^{1-Y_i} \right]$$

Logistic regression: a probabilistic version of classification loss

If a classifier $f(\mathbf{x}_i\beta) \in (0,1)$ provides a probability of $Y_i = 1$, $\hat{p}(Y_i|\mathbf{x}_i,\beta)$:

Bernoulli likelihood:

$$\prod_{i=1}^{n} f^{Y_i}(1-f)^{1-Y_i}$$

We can use negative log-likelihood as a "softer" version classification loss

$$L = \sum_{i=1}^{n} Y_i \log \overset{\text{what is this?}}{\frac{1-f(\mathbf{x}_i\beta)}{f(\mathbf{x}_i\beta)}} - \underset{\text{What if } f \to 1\text{?}}{\log(1-f(\mathbf{x}_i\beta))}$$

Understanding loss functions (soft vs. hard classification)

Soft classification loss

Given a classifier f outputs out class label probability $\in (0,1)$

$$L_n = \sum_{i=1}^{n} Y_i \log \overbrace{\frac{1 - f(\mathbf{x}_i\beta)}{f(\mathbf{x}_i\beta)}}^{\text{mistake odds ratio}} \underbrace{- \log(1 - f(\mathbf{x}_i\beta))}_{\text{will try to predict } f=0}$$

Total "mistake" log-odds ratio

Classification loss

Given a classifier spits out class label, e.g., $\{0,1\}$,

$$L_n = \frac{1}{n}\sum_{i=1}^{n} I\left\{ \underbrace{y_i}_{\text{observed}} \neq \underbrace{f(\mathbf{x}_i\beta)}_{\text{predicted}} \right\}$$

Average frequency of a wrong answer by the classifier.

Logistic loss function

Minimize this with respect to β:

$$L_n = \sum_{i=1}^{n} \left[-Y_i \overbrace{\sum_{k=1}^{p} X_{ik}\beta_k}^{\text{log-odds}} \underbrace{+ \log\left(1 + e^{\sum_{k=1}^{p} X_{ik}\beta_k}\right)}_{\text{"price" for the positive}} \right]$$

$\iff$

maximize the likelihood

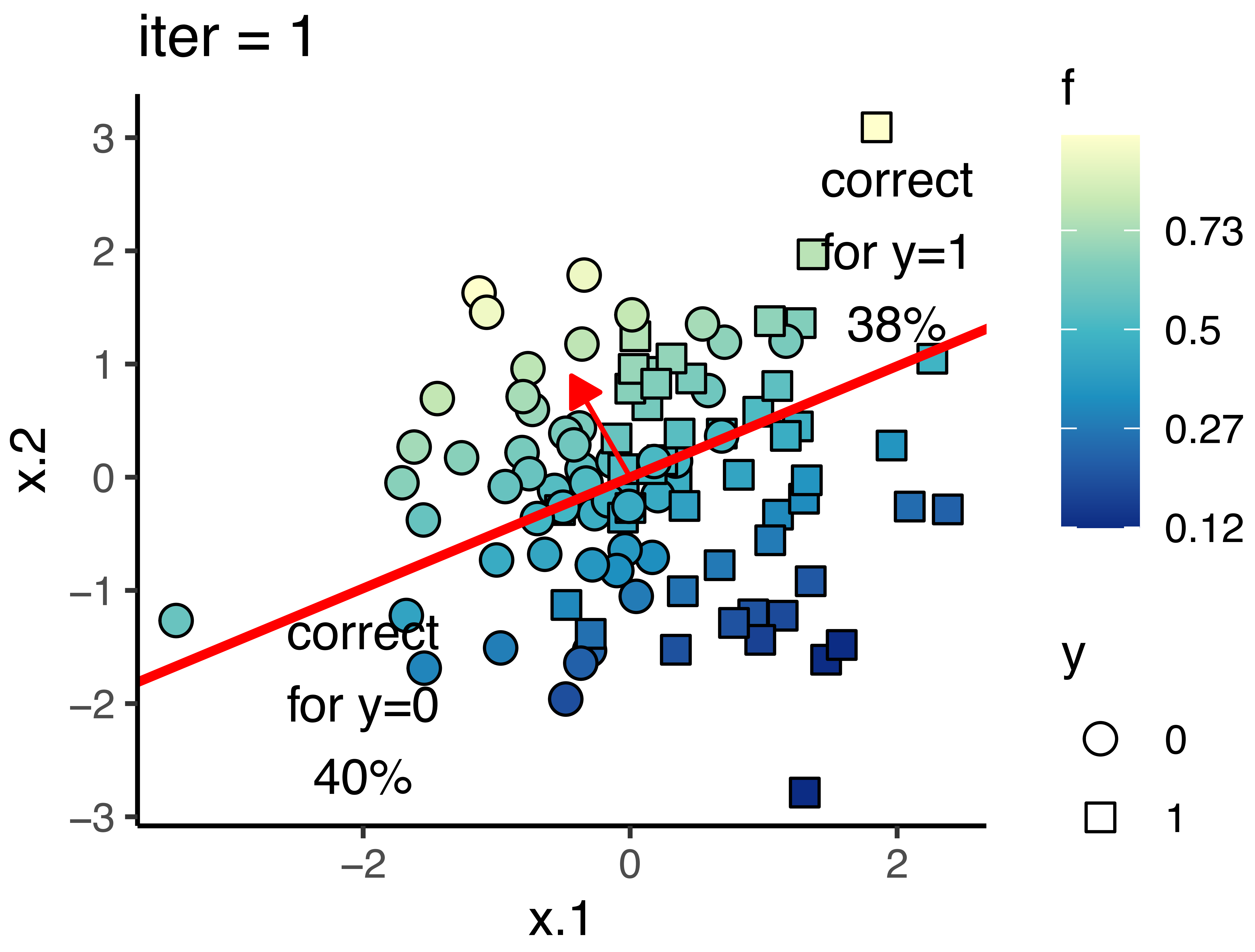
$$\mathcal{L}_n = \sum_{i=1}^{n} \left[Y_i \sum_{k=1}^{p} X_{ik}\beta_k - \log\left(1 + e^{\sum_{k=1}^{p} X_{ik}\beta_k}\right) \right]$$

A classification rule

Classifier

$$\hat{Y}_i = \begin{cases} 1 & \sum_{k=1}^{p} X_{ik}\beta_k > 0 \\ 0 & \sum_{k=1}^{p} X_{ik}\beta_k \leq 0 \end{cases}$$

Binary classification in action



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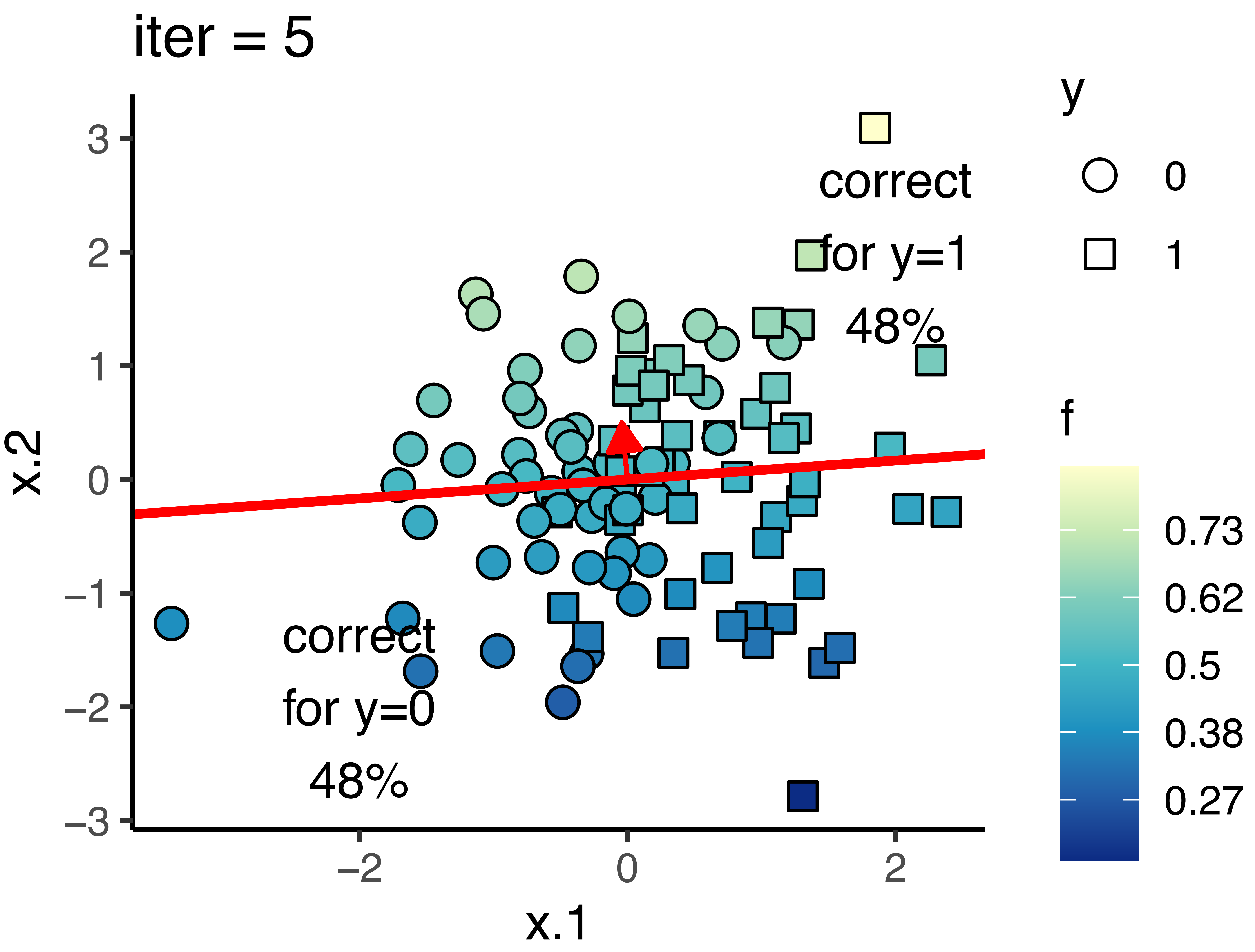

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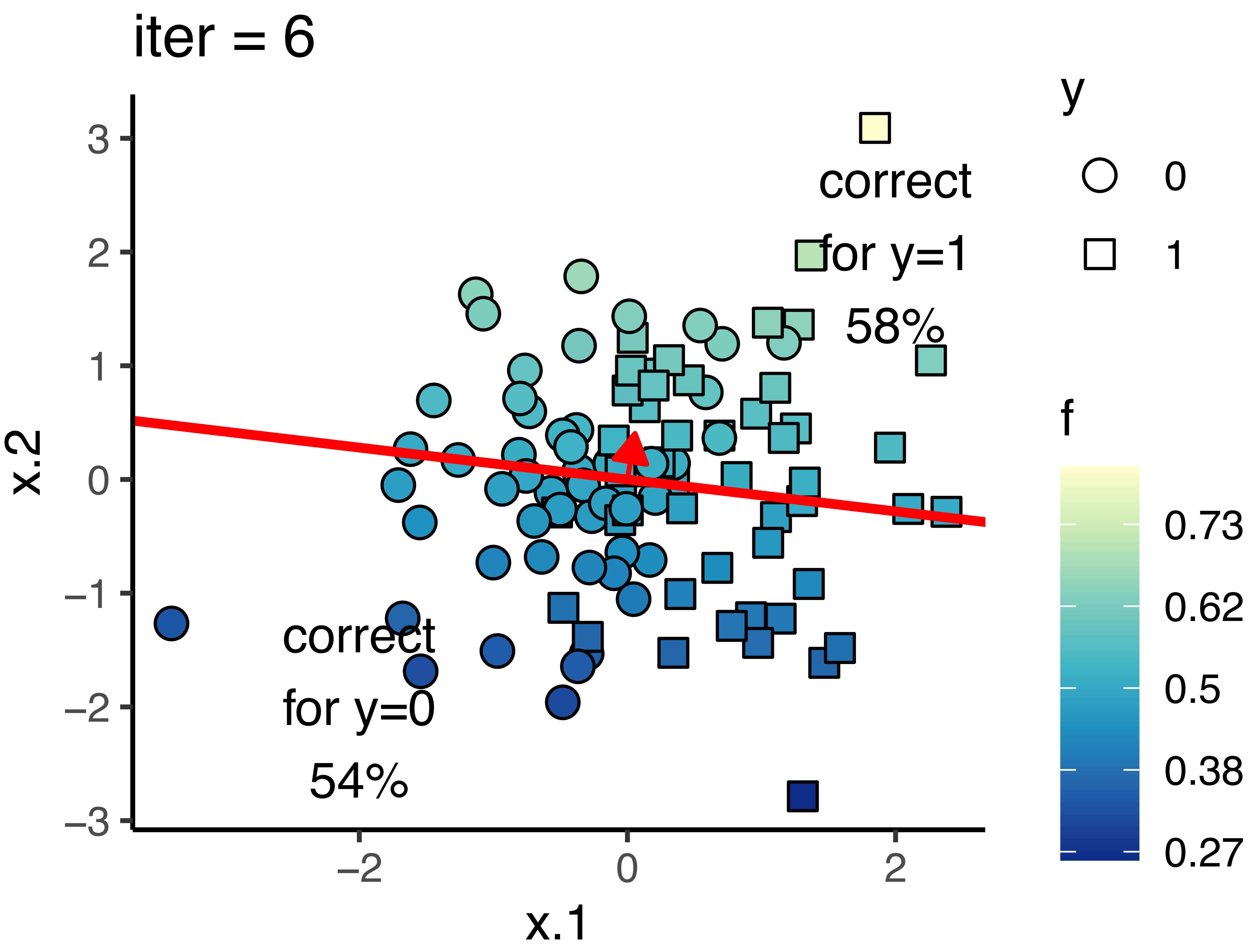

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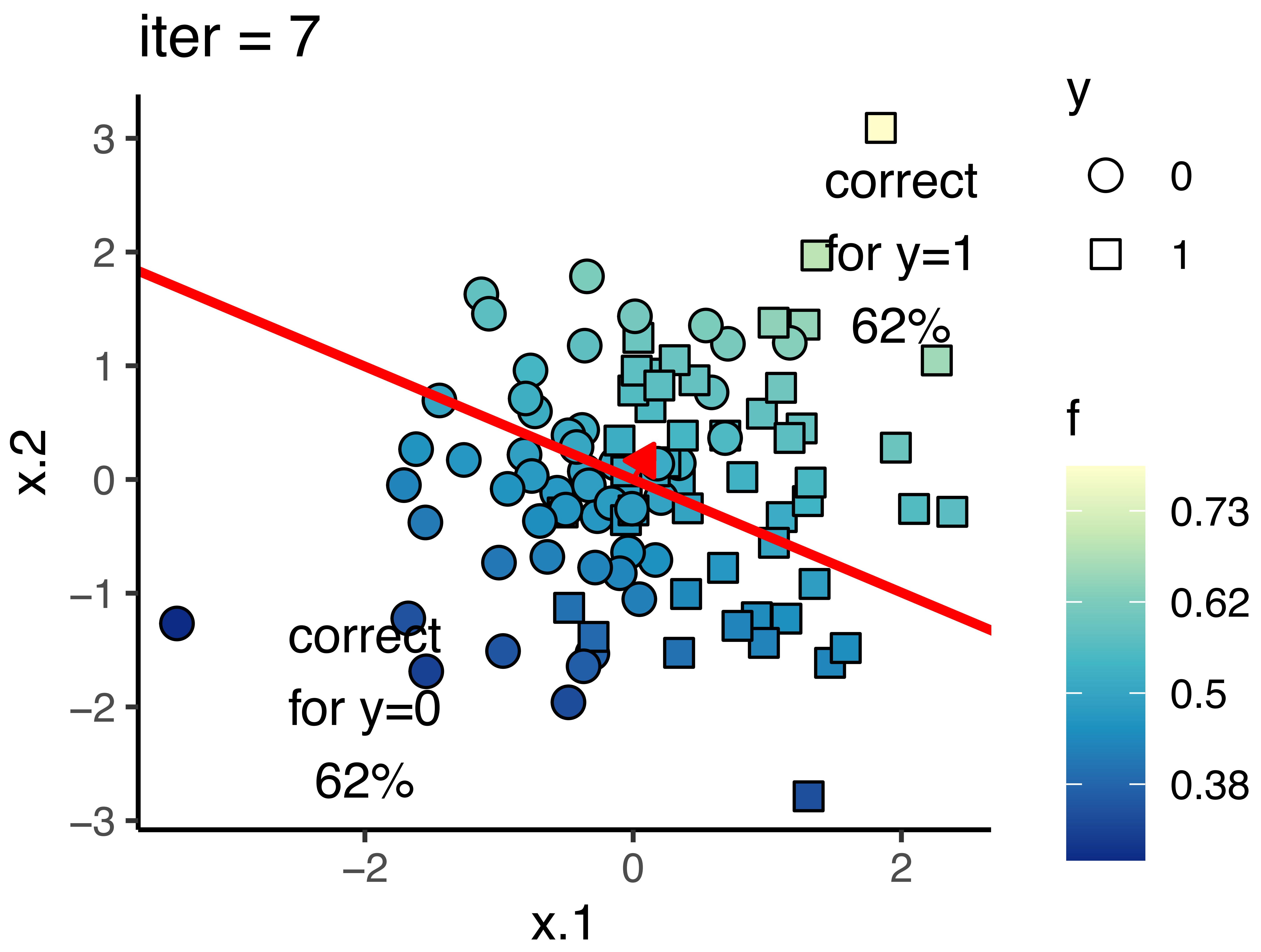

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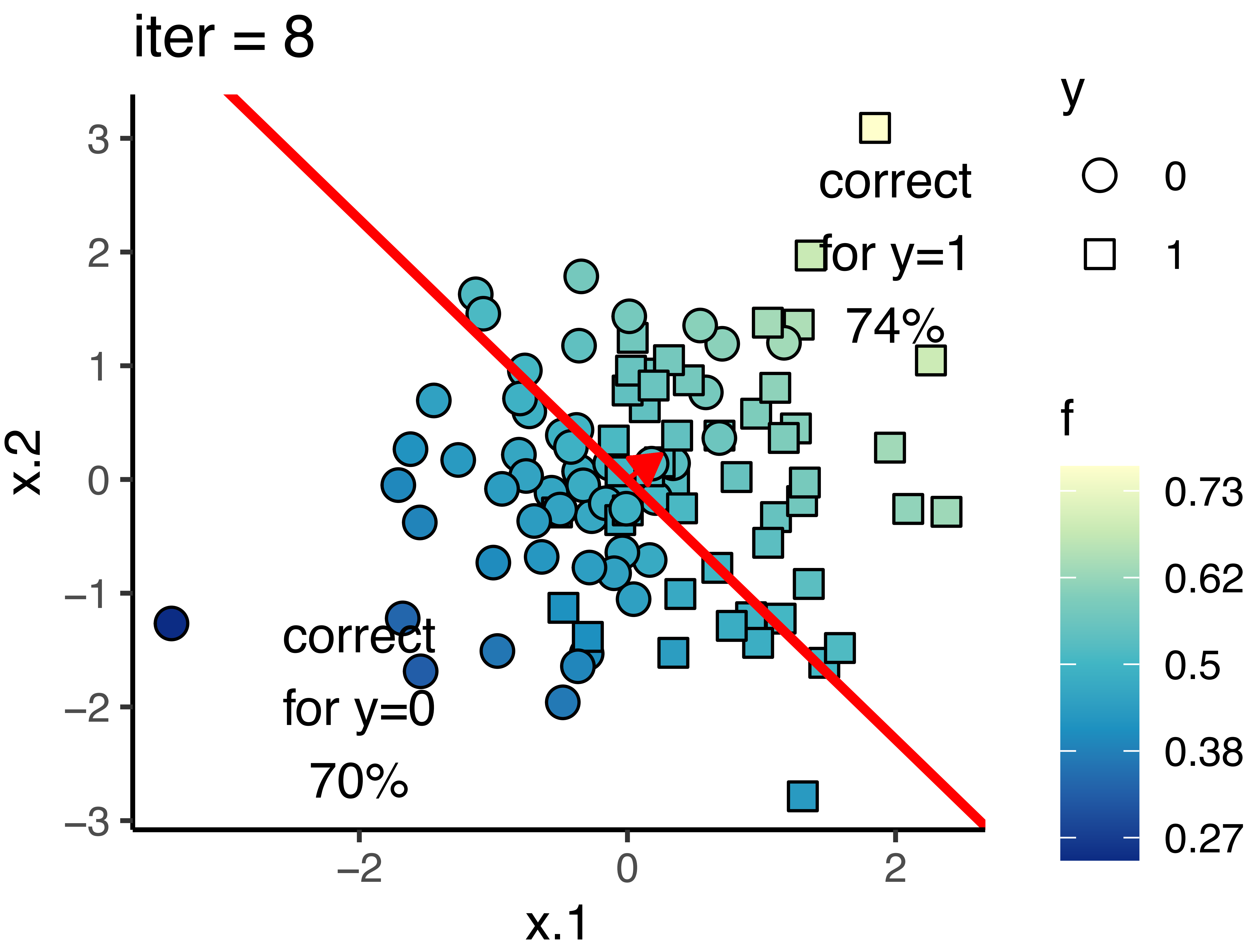

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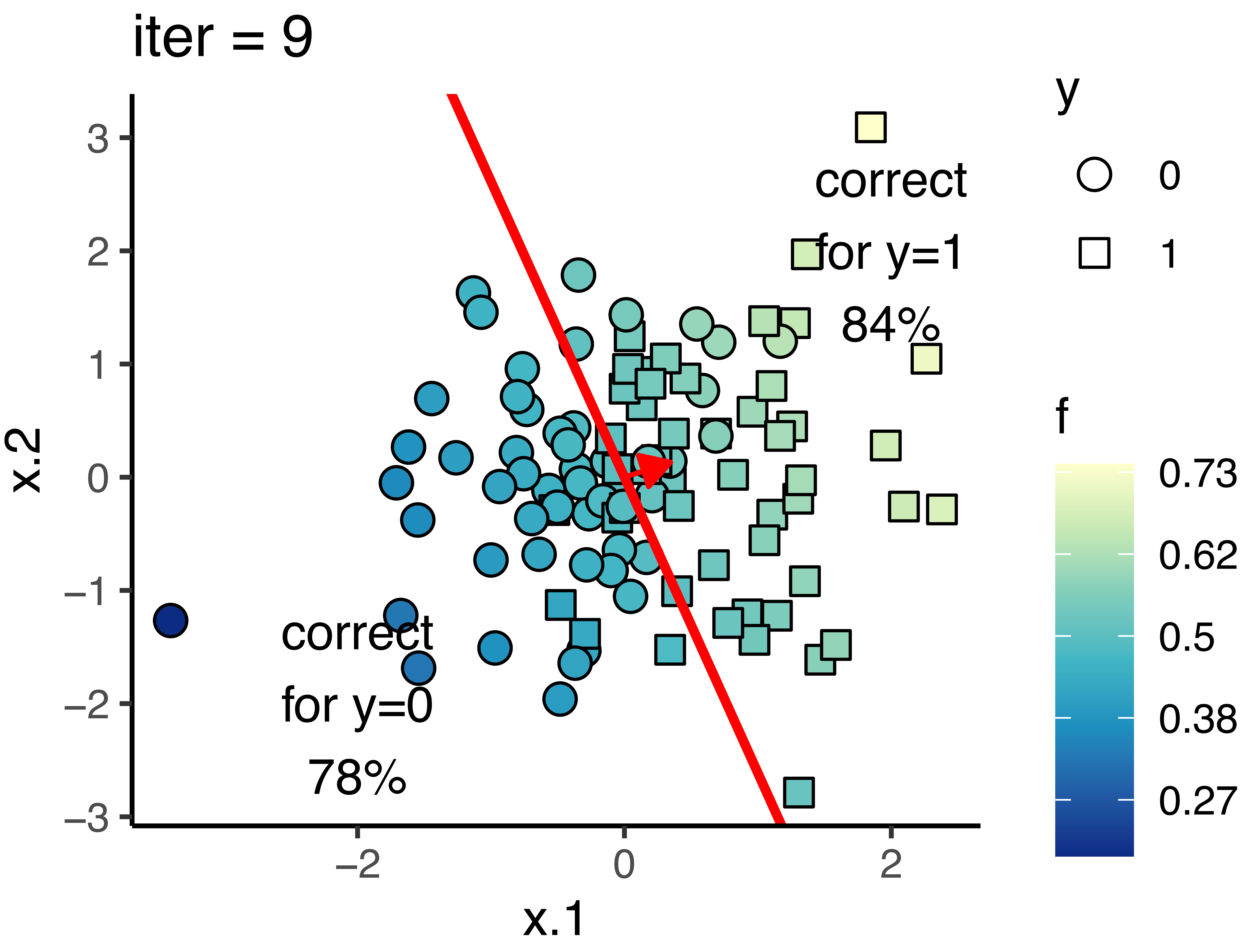

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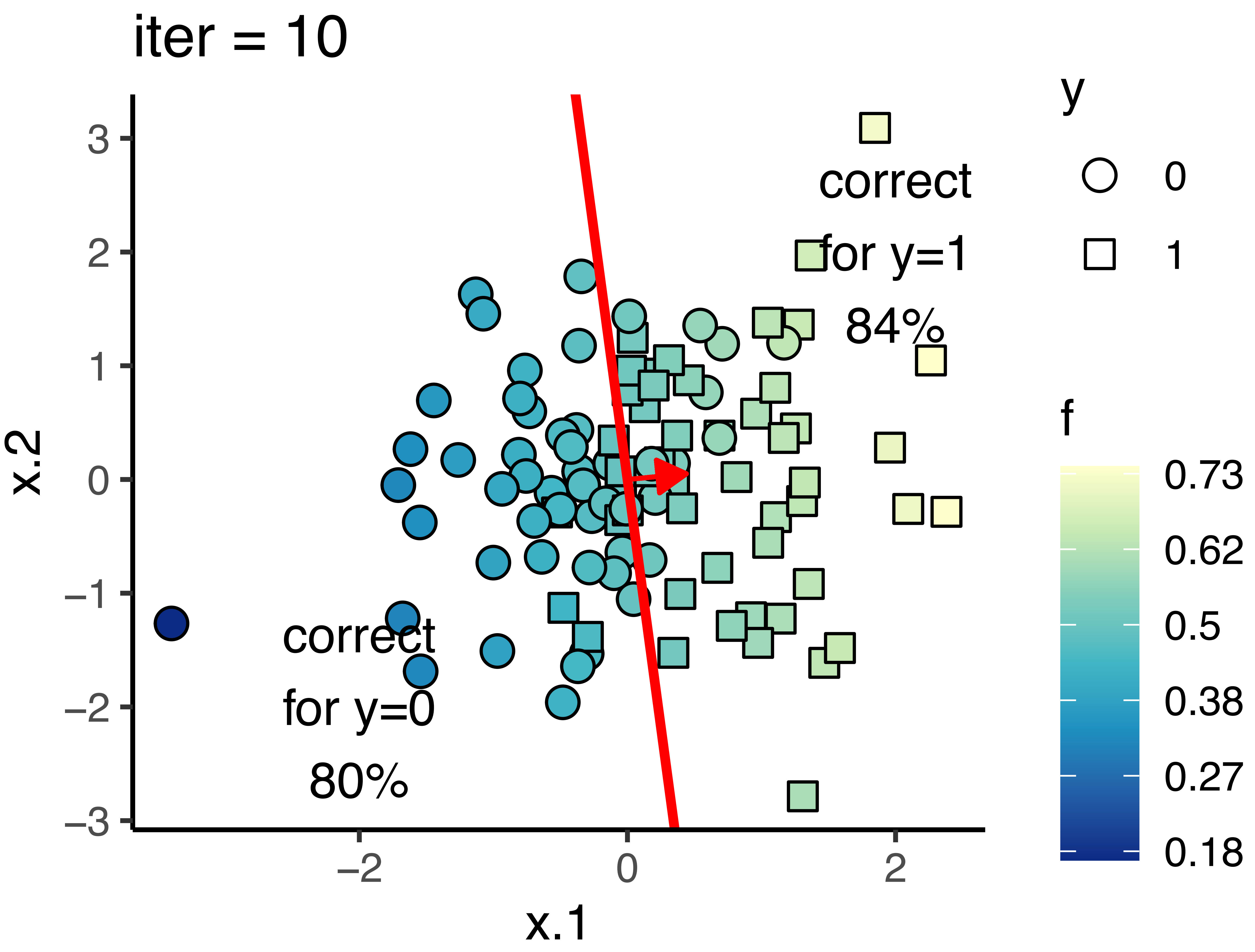

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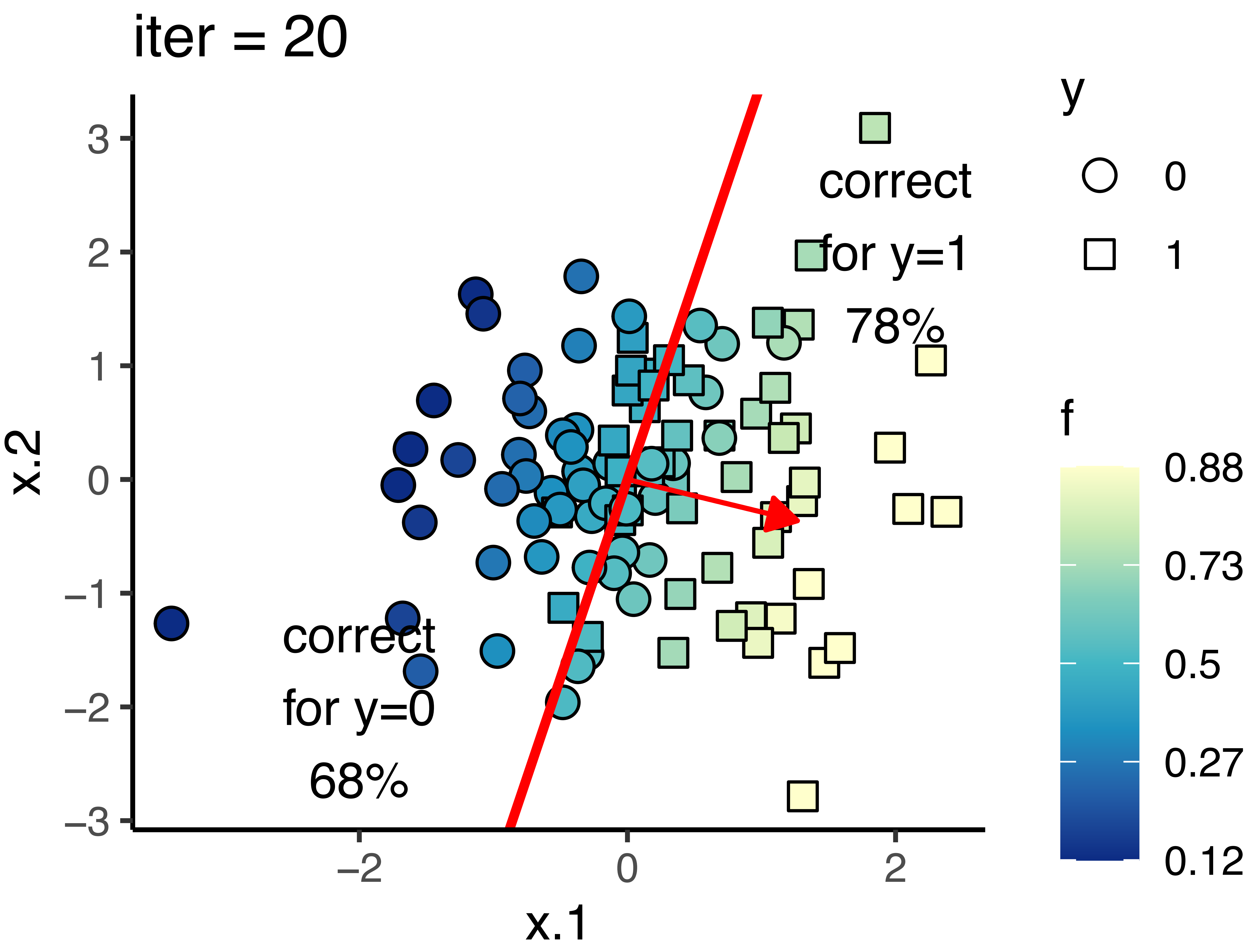

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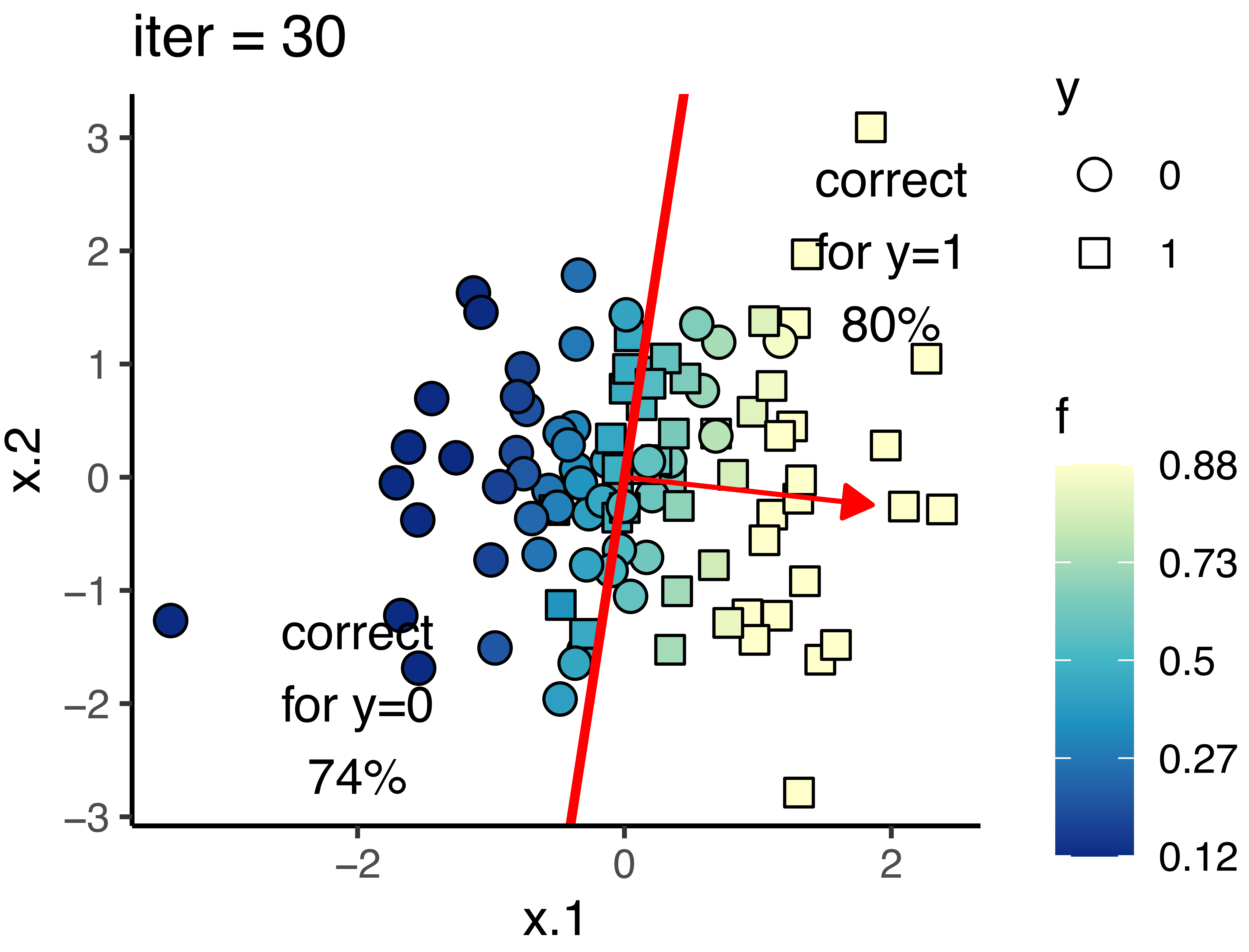

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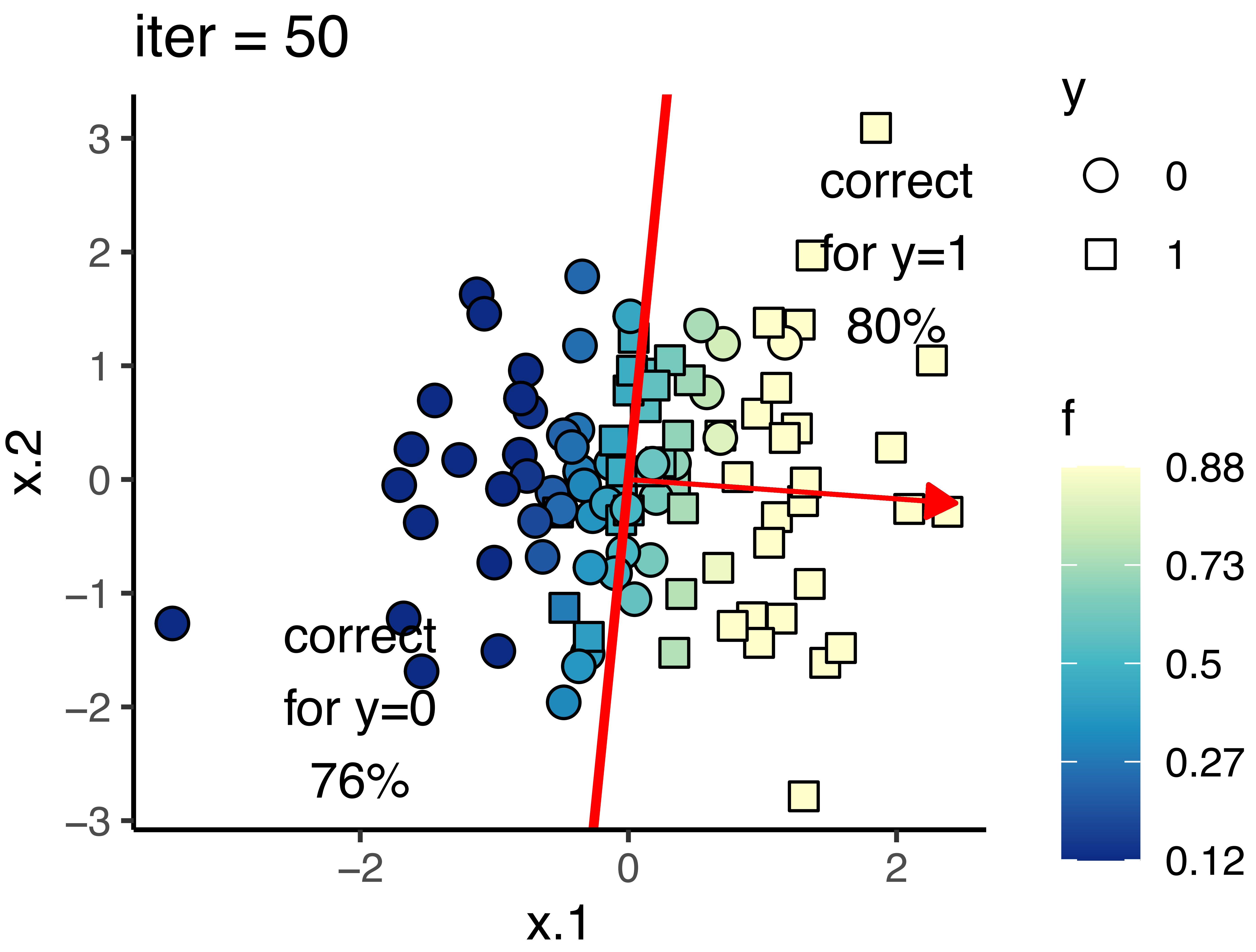

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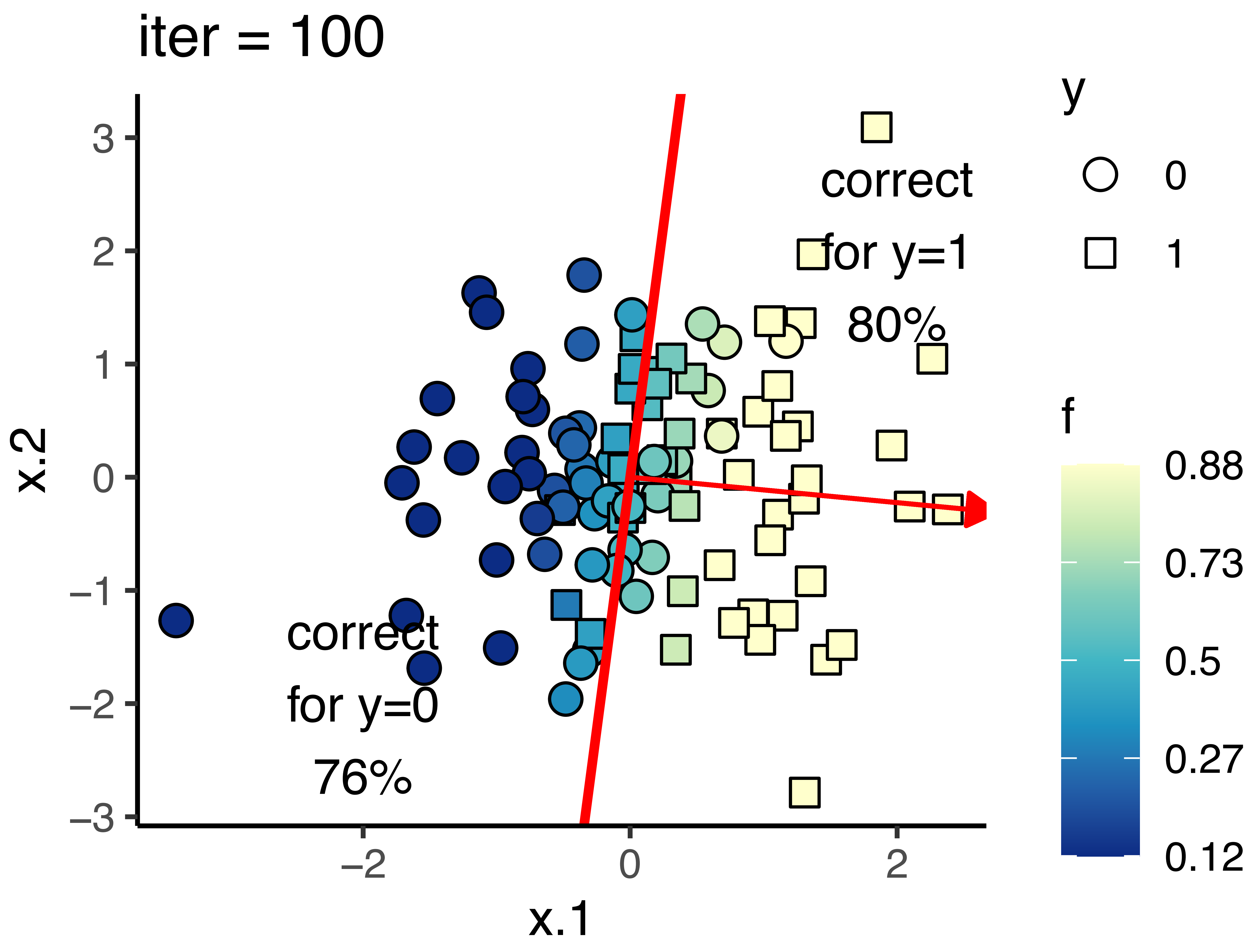

Today's lecture

General discussions on supervised learning

Classification with a decision rule

Generalized linear model

Generative Modelling approach

Other Methods

Revisit logistic regression as a "linear" model

(blurring the distinction between regression and classification)

A **linear** combination of features:

$$\sum_{k=1}^{p} X_{ik}\beta_k$$

Revisit logistic regression as a "linear" model

(blurring the distinction between regression and classification)

A **linear** combination of features:

$$\sum_{k=1}^{p} X_{ik}\beta_k$$

Letting $\eta_i = \sum_{k=1}^{p} X_{ik}\beta_k$, we define log-likelihood as:

$$\mathcal{L} = \sum_{i=1}^{n} \log p(Y_i|\eta_i) = \sum_{i=1}^{n} \sigma(\eta_i) + (1 - Y_i)\sigma(-\eta_i)$$

where $\sigma(z) = 1/(1 + \exp(-z))$.

Many interesting data types can be modelled as a GLM

A linear combination of features

$$\eta_i = \sum_{k=1}^{p} X_{ik}\beta_k$$

can be morphed to many different types of Y:

$$Y_i \sim p(Y_i | \eta_i)$$

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Poisson

$$p(Y_i|\lambda_i) = \frac{\lambda_i^{Y_i} e^{-\lambda_i}}{Y_i!}$$

where $\lambda_i = \exp(\eta_i)$

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where $\lambda_i = \exp(\eta_i)$

Gamma

$$p(Y_i|\mu_i, \phi) = \frac{(\phi\mu_i)^{-1/\phi}}{\Gamma(1/\phi)} Y_i^{1/\phi-1} e^{-Y_i/\mu_i\phi}$$

where $\mu_i = \exp(\eta_i)$ and ϕ is an overdispersion parameter

Negative Binomial GLM: directly modelling RNA-seq count

Poisson and Gamma distributions are the building blocks of NB.

$$p(Y_i|\mu_i, \phi) \;=\; \int \overbrace{p(Y_i|\lambda_i)}^{\text{Poisson}} \underbrace{p(\lambda_i|\mu_i, \phi)}_{\text{Gamma}} \, d\lambda_i$$

where we model

$$\mu_i = \exp\left(\sum_{k=1}^{p} X_{ik}\beta_k\right).$$

Negative Binomial GLM: directly modelling RNA-seq count

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$$
\begin{aligned}
p(Y_i|\mu_i,\phi) &= \int \overbrace{p(Y_i|\lambda_i)}^{\text{Poisson}} \underbrace{p(\lambda_i|\mu_i,\phi)}_{\text{Gamma}} d\lambda_i \\
&= \underbrace{\frac{\Gamma(Y_i+1/\phi)}{\Gamma(Y_i+1)\Gamma(1/\phi)}}_{\text{negative binomial}} \underbrace{\left(\frac{\mu_i}{1/\phi+\mu_i}\right)^{Y_i}}_{\text{success rate}} \underbrace{\left(\frac{1/\phi}{1/\phi+\mu_i}\right)^{1/\phi}}_{\text{failure rate}}
\end{aligned}
$$

where we model

$$
\mu_i = \exp\left(\sum_{k=1}^{p} X_{ik}\beta_k\right).
$$

Negative Binomial GLM: directly modelling RNA-seq count

- Y: number of successfully "observed" reads in RNA-seq (∼targeting)
- r: number of permitted "dropped" reads until Y observed (∼budget)
- ρ: success rate

$$p(Y_i|\mu_i, \phi) = \underbrace{\binom{Y_i + r - 1}{Y_i}}_{\text{negative binomial}} \underbrace{\rho_i^{Y_i}}_{\text{success rate}} \underbrace{(1 - \rho_i)^r}_{\text{drop rate}}$$

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\text{or} \quad &= \mathrm{NB}(Y_i | \text{mean} = \mu_i, \text{overdispersion} = \phi)
\end{aligned}
$$

We can check:

mean: $\mathbb{E}[Y_i | r, \rho] = \rho r / (1 - \rho) = \mu_i$

variance: $\mathbb{V}[Y_i | r, \rho] = \rho r / (1 - \rho)^2 = \mu_i + \mu_i^2 \phi$ (overdispersed mean-variance)

Four Steps for Supervised Learning

1. Gather some training data (this is a part of research!):
2. Write down a model (classifier) $f : \mathcal{X} \to \mathcal{Y}$
3. Fit the model to the training data
4. Use the model

https://github.com/STAT540-UBC/lectures/blob/main/lect17-ml_intro/lect17-supervised-part1.Rmd

Step 1. Cell type deconvolution data

Data set

- Human pancreatic islet gene expression data: GSE50244
- Single cell RNA-seq data in the same tissue: E-MTAB-5061
- A processed data set is available here: https://github.com/xuranw/MuSiC/tree/master/vignettes/data

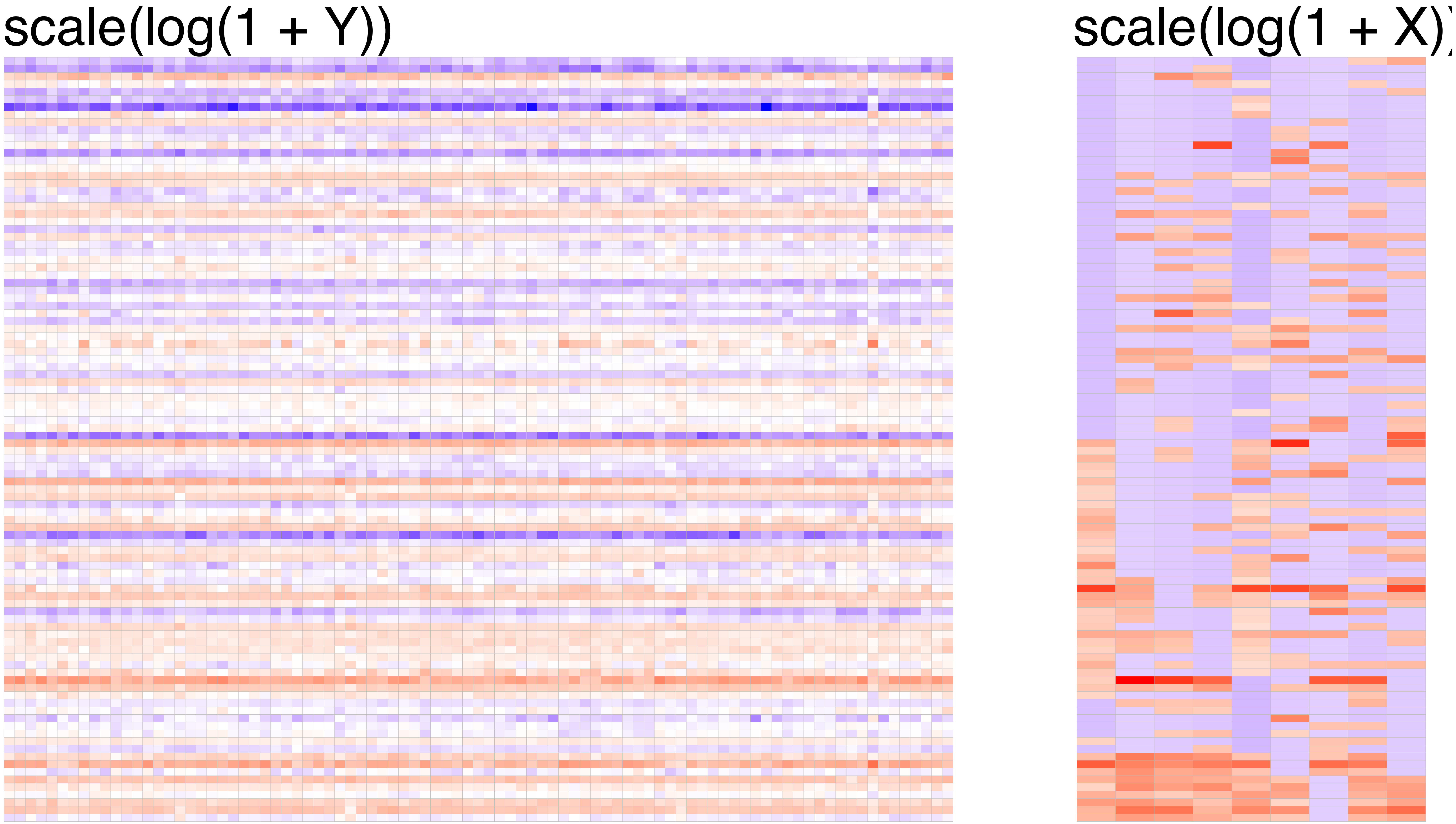
Problem definition

- $\mathbf{y}$: bulk gene expression (gene $\times$ sample)
- X: cell-type-specific single-cell expression (gene $\times$ cell type)

Goal

1. Fit a model regressing the bulk profile $\mathbf{y}_i$ of a sample i on the single-cell-type-specific matrix X.
2. What are the estimated cell type fractions in the bulk sample?

Step 1. (show the data)



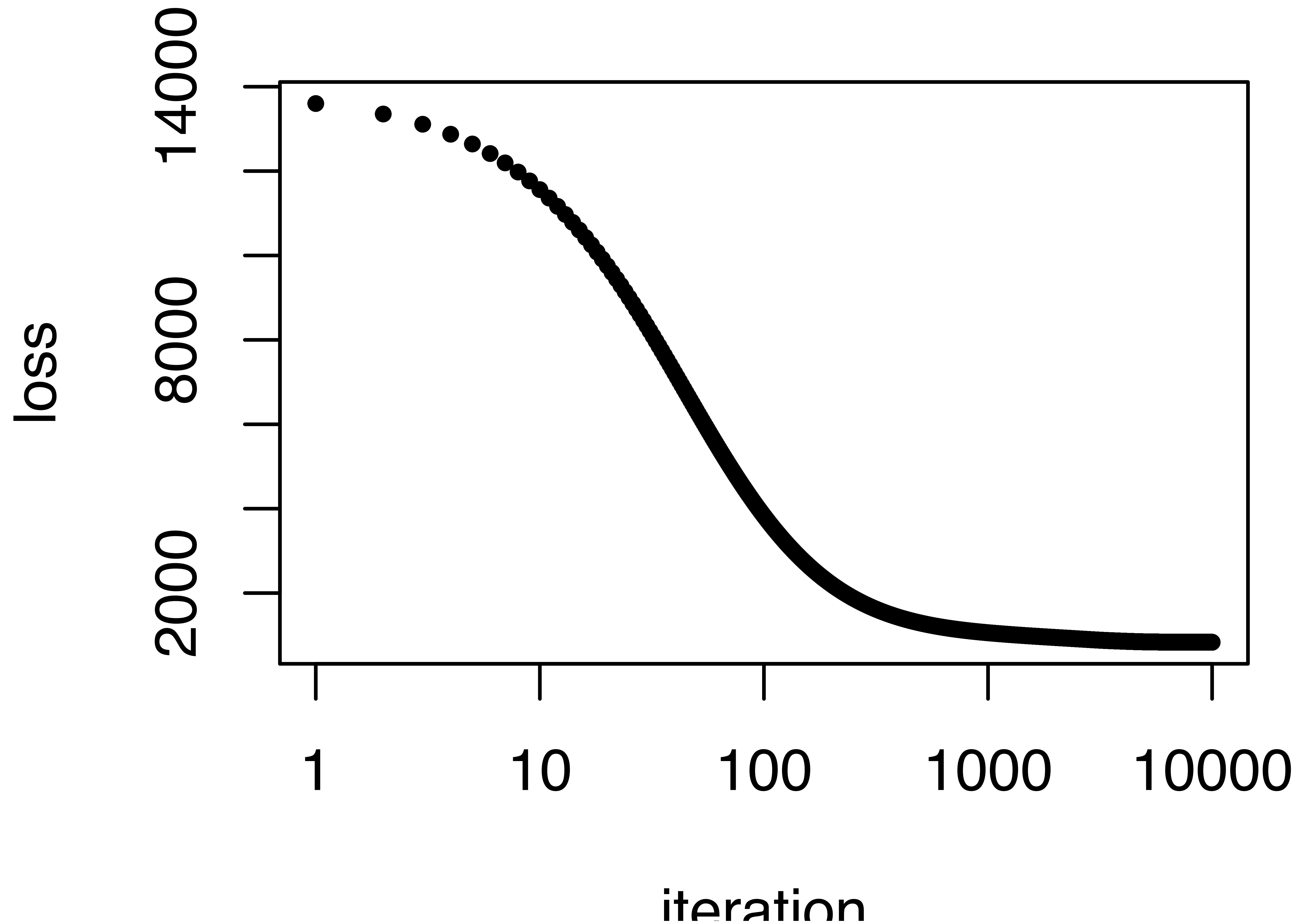
Step 2. NB GLM for the cell type deconvolution problem

Q: Can we estimate cell type fractions in tissue-level *bulk* data?

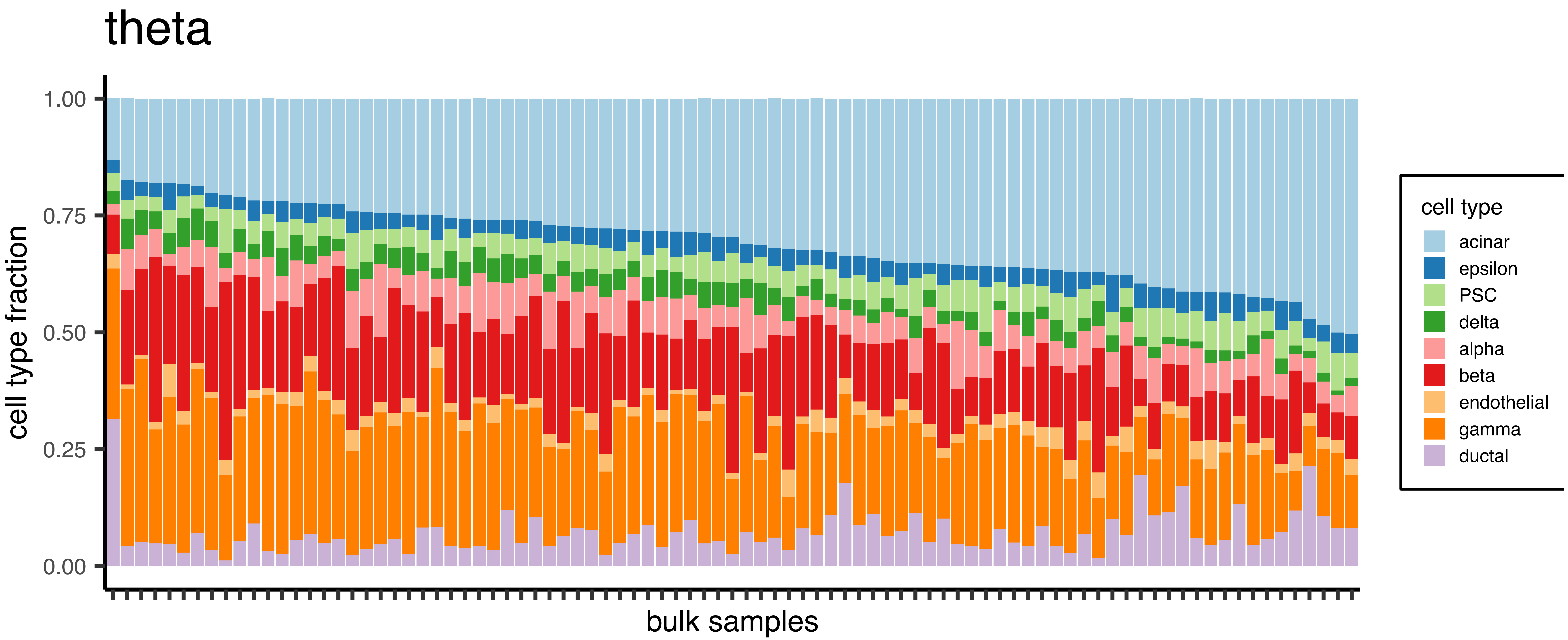
$$\overset{\text{bulk}}{\mathbf{y}_i} \sim \mathrm{NB}\left(\text{mean} = \overset{\text{scale factor}}{s_i} \underbrace{\sum_t X_{gt}}_{\text{cell-type-sorted}} \overset{\text{GOAL}}{\theta_{ti}}, \text{overdispersion} = \phi\right)$$

- We use the same data set used in the vignette of MuSic package (Wang *et al.*, Nature Comm., 2019)

Step 3. Fit the model to the data



Step 4. Show the cell type fraction estimates



Today's lecture

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Other Methods

Discriminative vs. generative approach

- Y: class label/outcome, X: covariates/predictor variables

Discriminative learning

- Directly learn $p(Y|X)$

Generative learning

- First learn $p(X|Y)$
- Apply **Bayes** rule: $p(Y|X) \propto p(X|Y)p(Y)$

- If we have domain-specific knowledge, $p(X|Y)$, a generative-modelling approach can be more powerful.
- If our focus is solely on classification, a discriminative learning approach usually outperforms with small to moderate sample size.

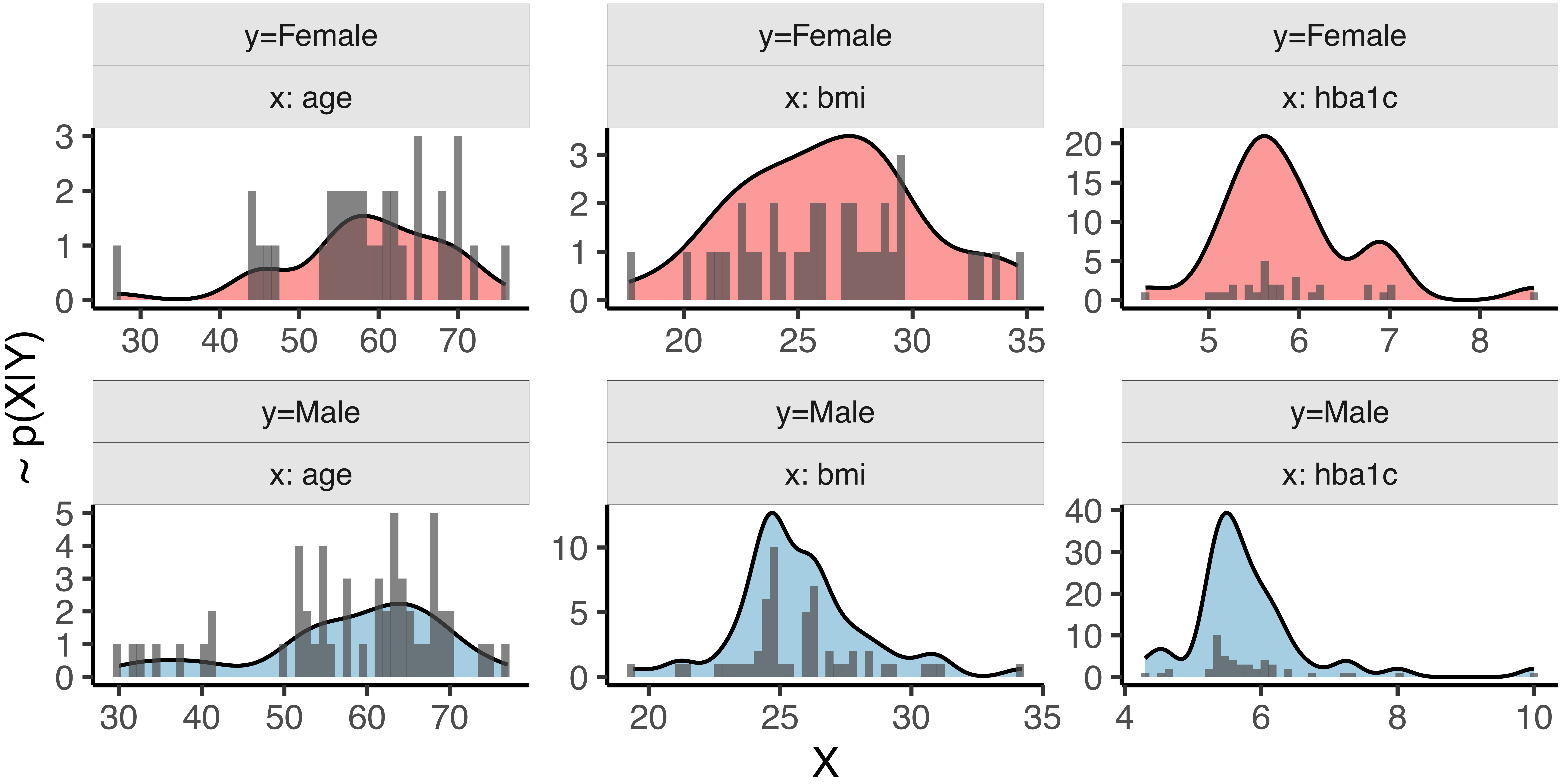
Naive Bayes Classifier: How do we estimate $P(X|Y)$?

If $\mathbf{x}_i = (X_{i1}, \ldots, X_{ip})$, how do we estimate $p(\mathbf{x}_i|Y_i = 1)$ or $p(\mathbf{x}_i|Y_i = 0)$?

$$p(X_{i1}, \ldots, X_{ip}|Y_i = y_i) \underset{\text{fully-factored}}{\approx} \prod_{k=1} p(X_{ik}|Y_i)$$

- Is this accurate?
- What have we missed?

Let's take an example from the pancreatic islet data (`GSE50244`).



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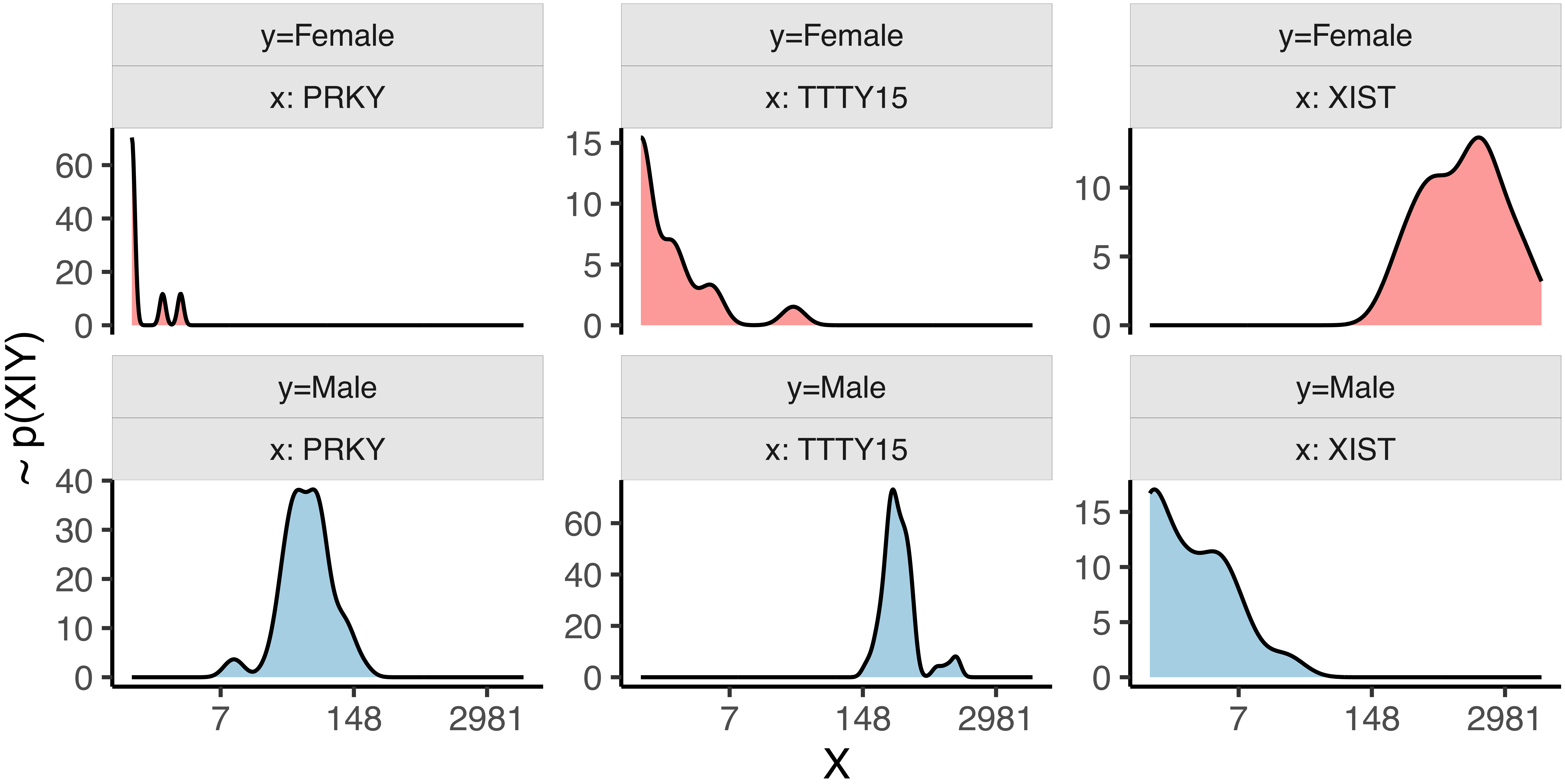
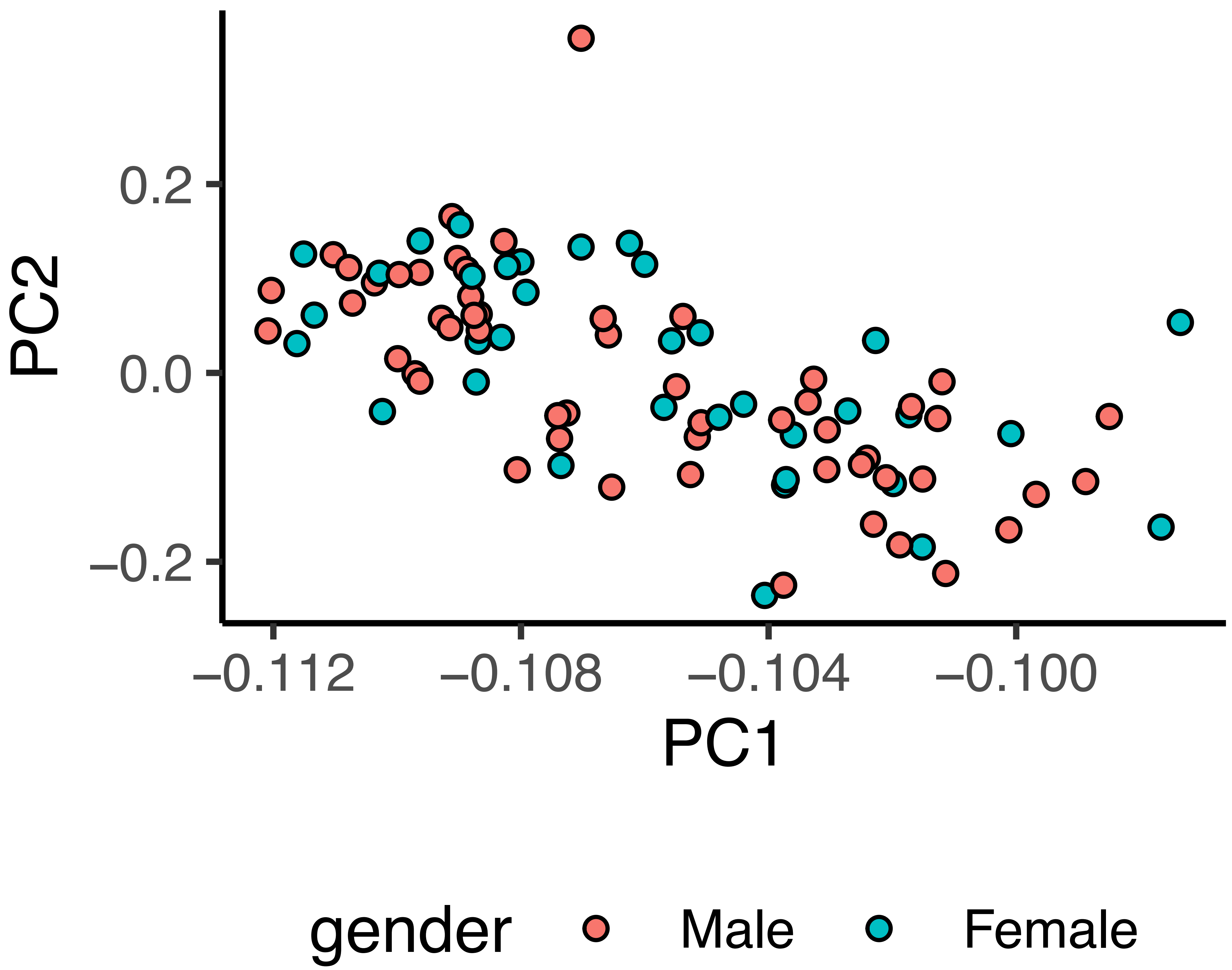
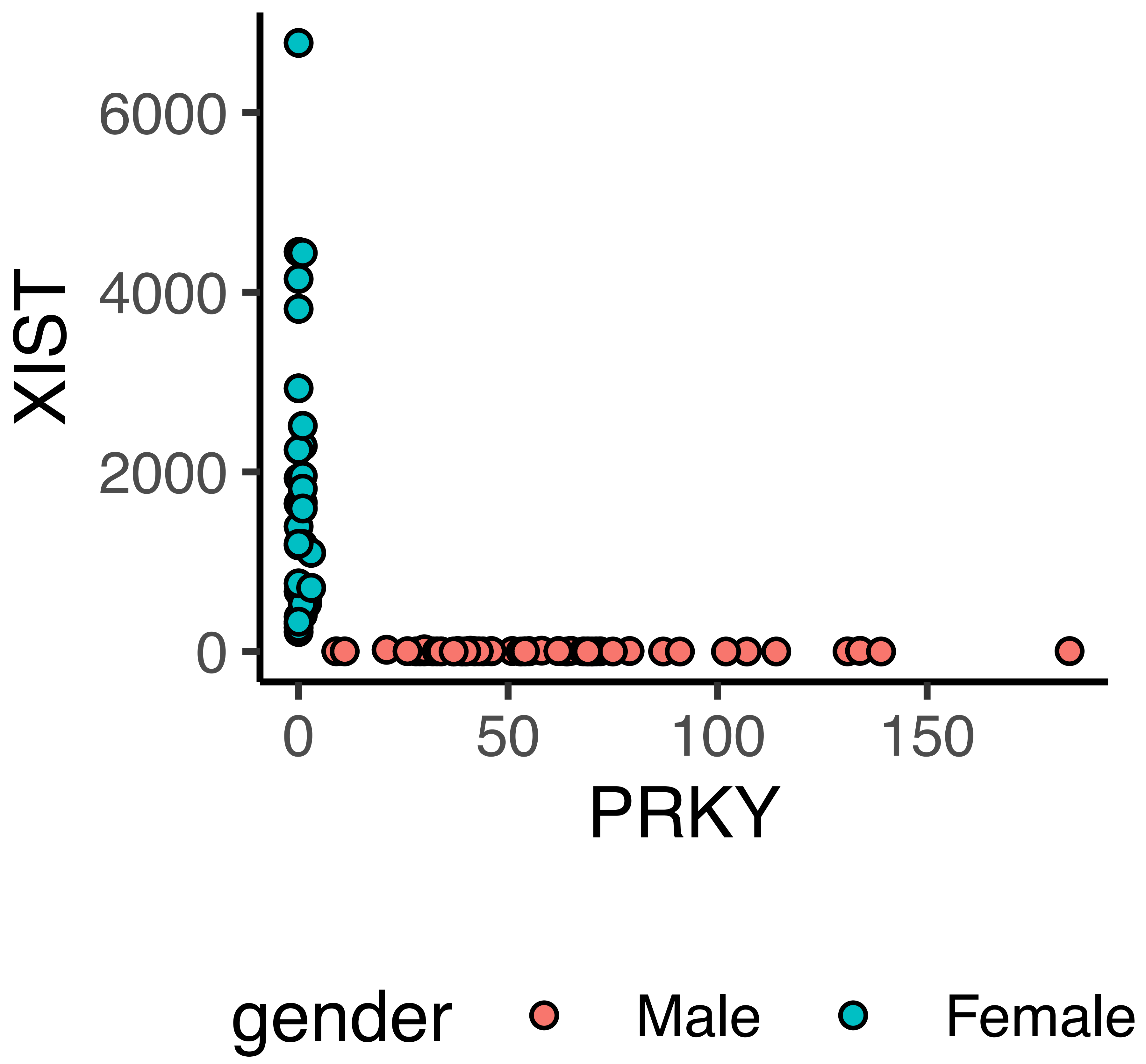


Not every gene can predict well



These genes are very informative



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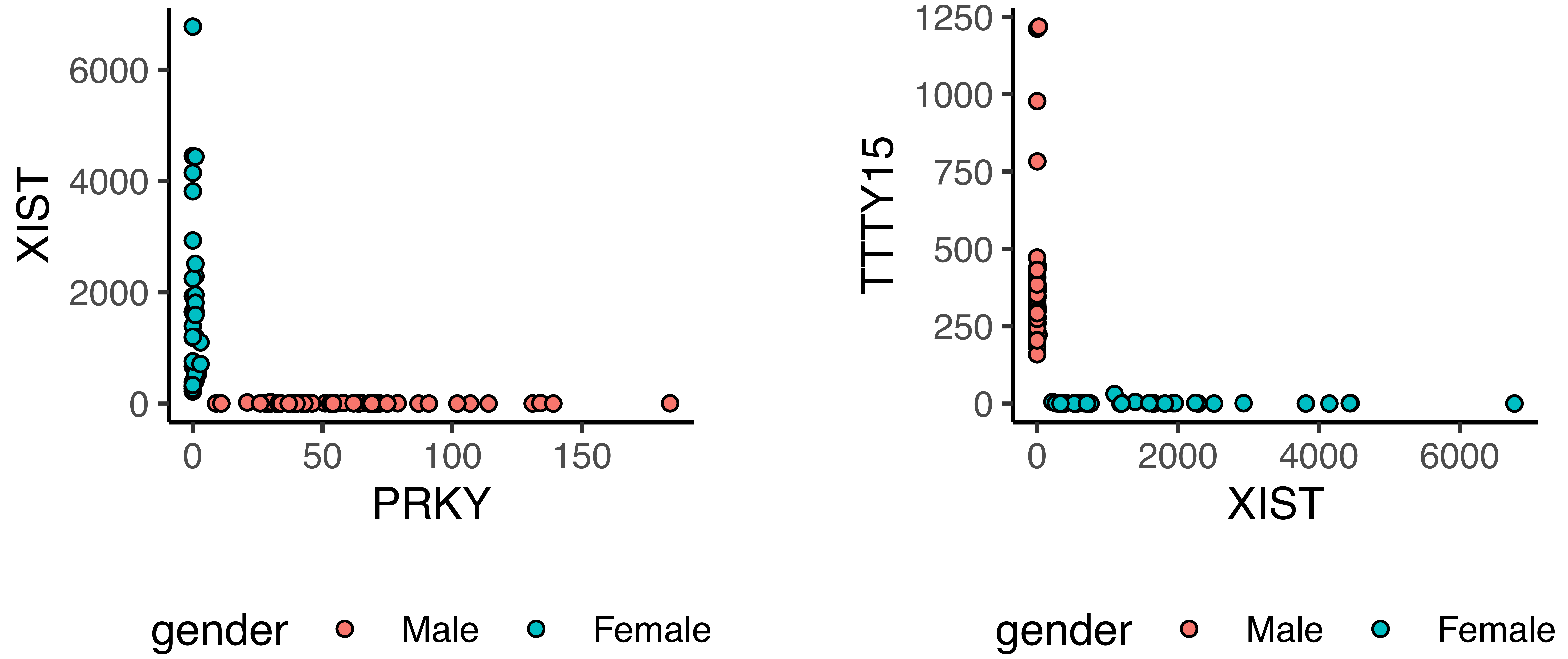

Naive Bayes Classifier

$$p(Y_i = 1|\mathbf{x}_i) \approx \frac{\overbrace{p(Y_i = 1)}^{\text{prior}} \overbrace{\prod_k \hat{p}(X_{ik}|\theta_{k1})}^{\text{fully-factored}}}{\sum_{c=0}^{1} p(Y_i = c) \prod_k \hat{p}(X_{ik}|\theta_{kc})}$$

- Prior can be $1/2$ if the class labels are balanced (or $1/K$ for K classes).

Naive Bayes Classifier

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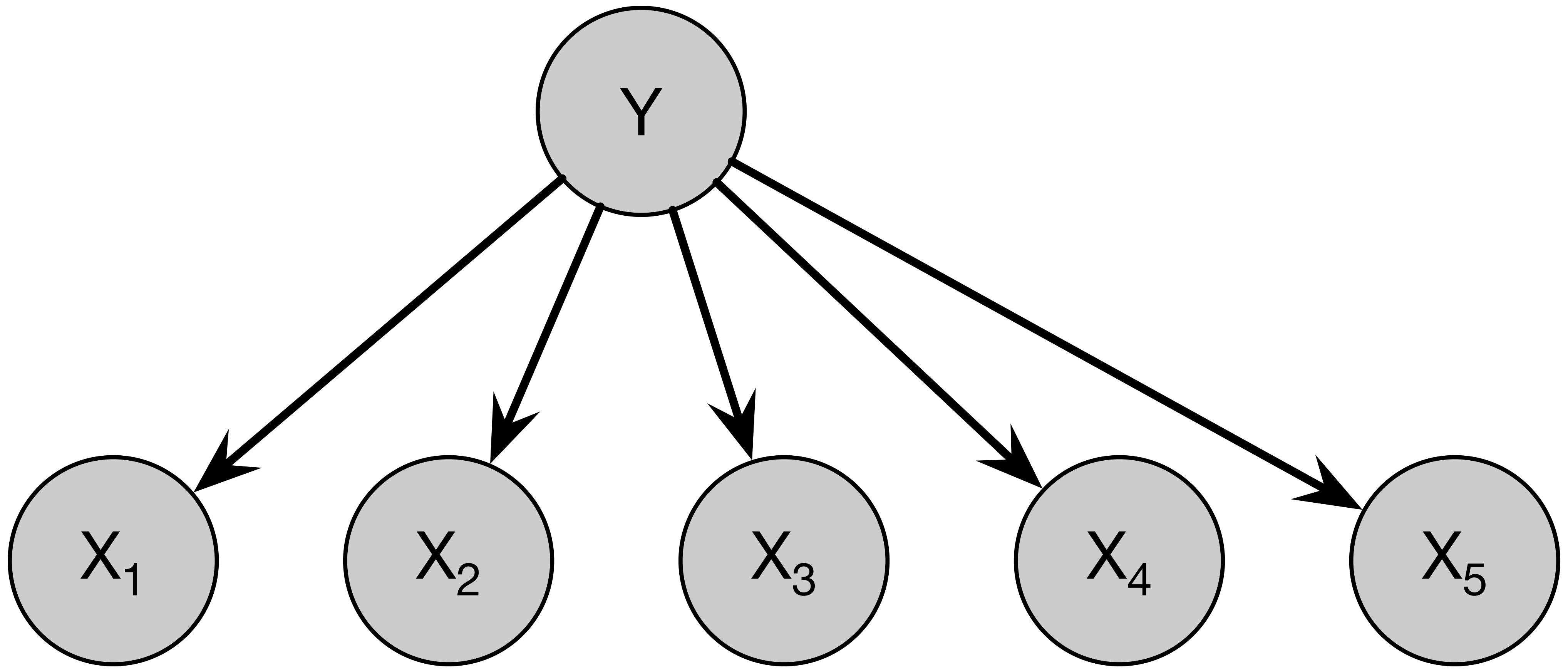
$$\approx \frac{p(Y_i = 1) \prod_k \overbrace{\mathcal{N}(X_{ik}|\mu_{k1}, \sigma_{k1}^2)}^{\text{Gaussian approximation}}}{\sum_{c=0}^{1} p(Y_i = c) \prod_k \underbrace{\mathcal{N}(X_{ik}|\mu_{kc}, \sigma_{kc}^2)}_{\text{Gaussian approximation}}}$$

- Prior can be $1/2$ if the class labels are balanced (or $1/K$ for K classes).

Can we improve Naive Bayes Classifier?



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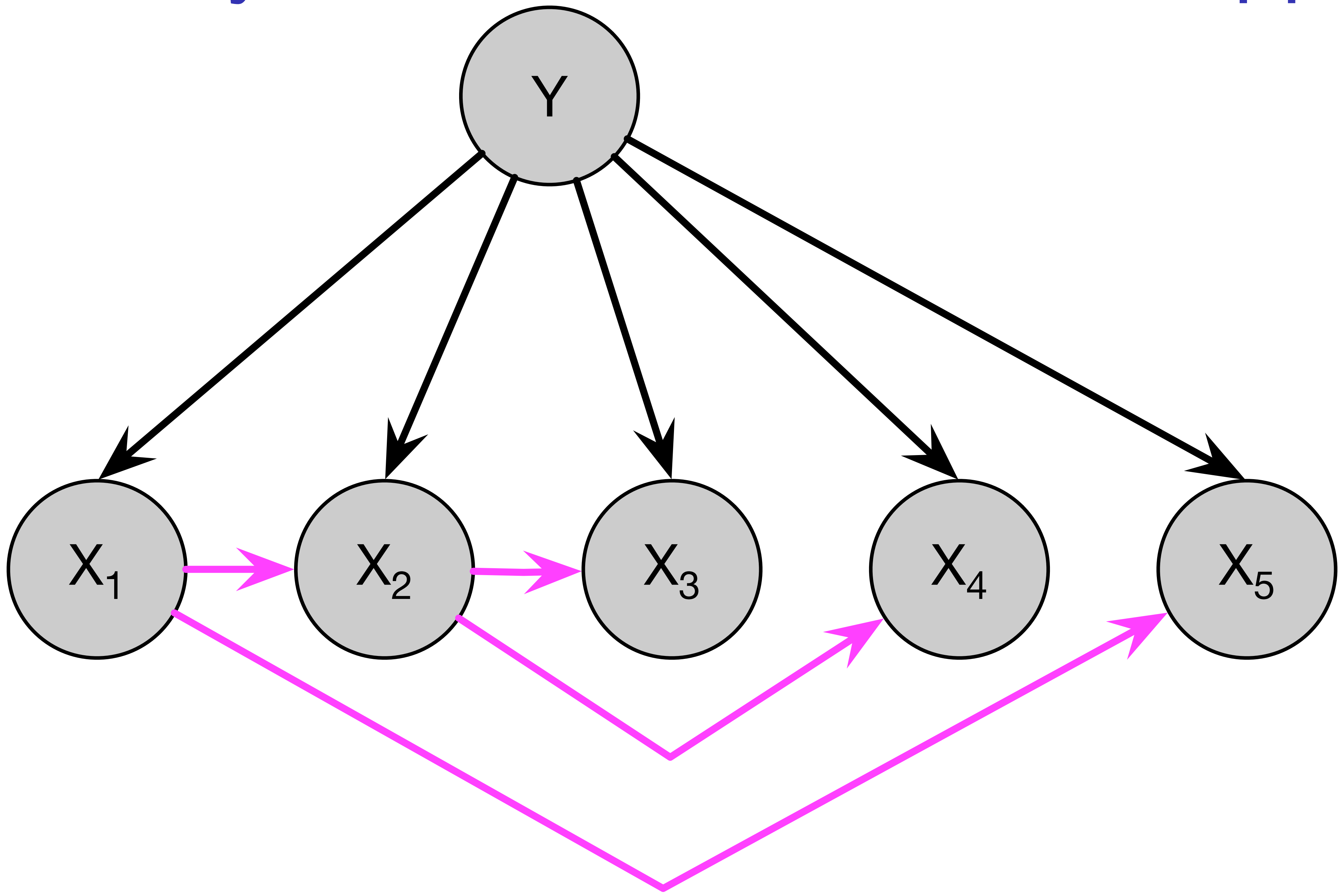
Tree-augmented Naive Bayes Classifier can better approximate $P(X|Y)$



$$p(Y_i = 1|\mathbf{x}_i) \approx \frac{\overbrace{p(Y_i = 1)}^{\text{prior}} \overbrace{\prod_k \hat{p}(X_{ik}|X_{i\mathsf{Pa}(k)}, \theta_{k1})}^{\text{tree-structured}}}{\sum_{c=0}^{1} p(Y_i = c) \prod_k \hat{p}(X_{ik}|X_{i\mathsf{Pa}(k)}, \theta_{kc})}$$

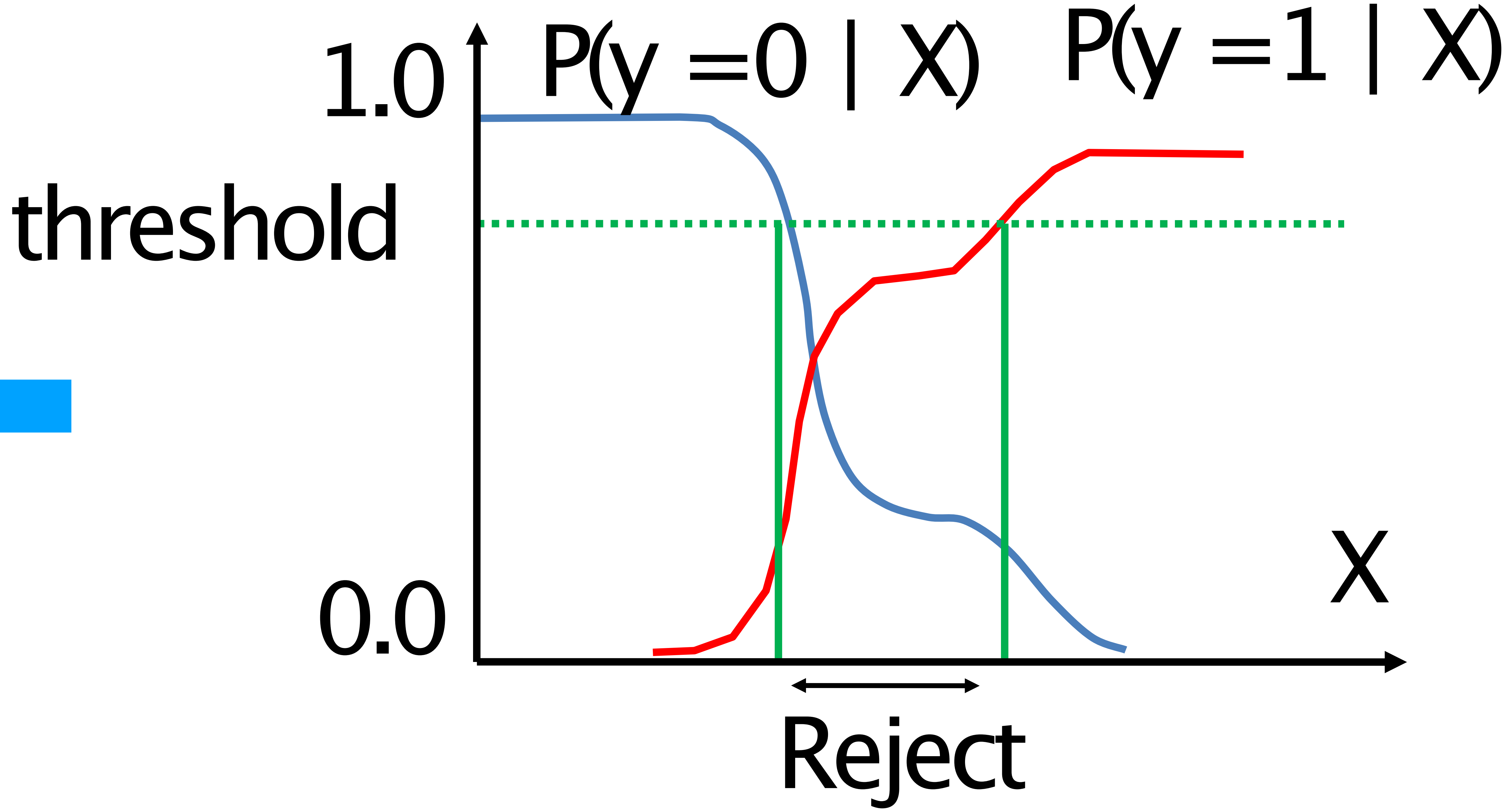
- Can we use prior knowledge, such as Gene Ontology?

Today's lecture

- **A Brief History of Machine Learning in Computational Biology**
  - What is ML? Why ML in Comp. Bio?
  - ML in many genomics problems
- **Supervised Statistical Learning 101**
  - Binary classification problem
  - Cell-type deconvolution example
  - Discriminative vs. Generative learning
- **Evaluation metrics**

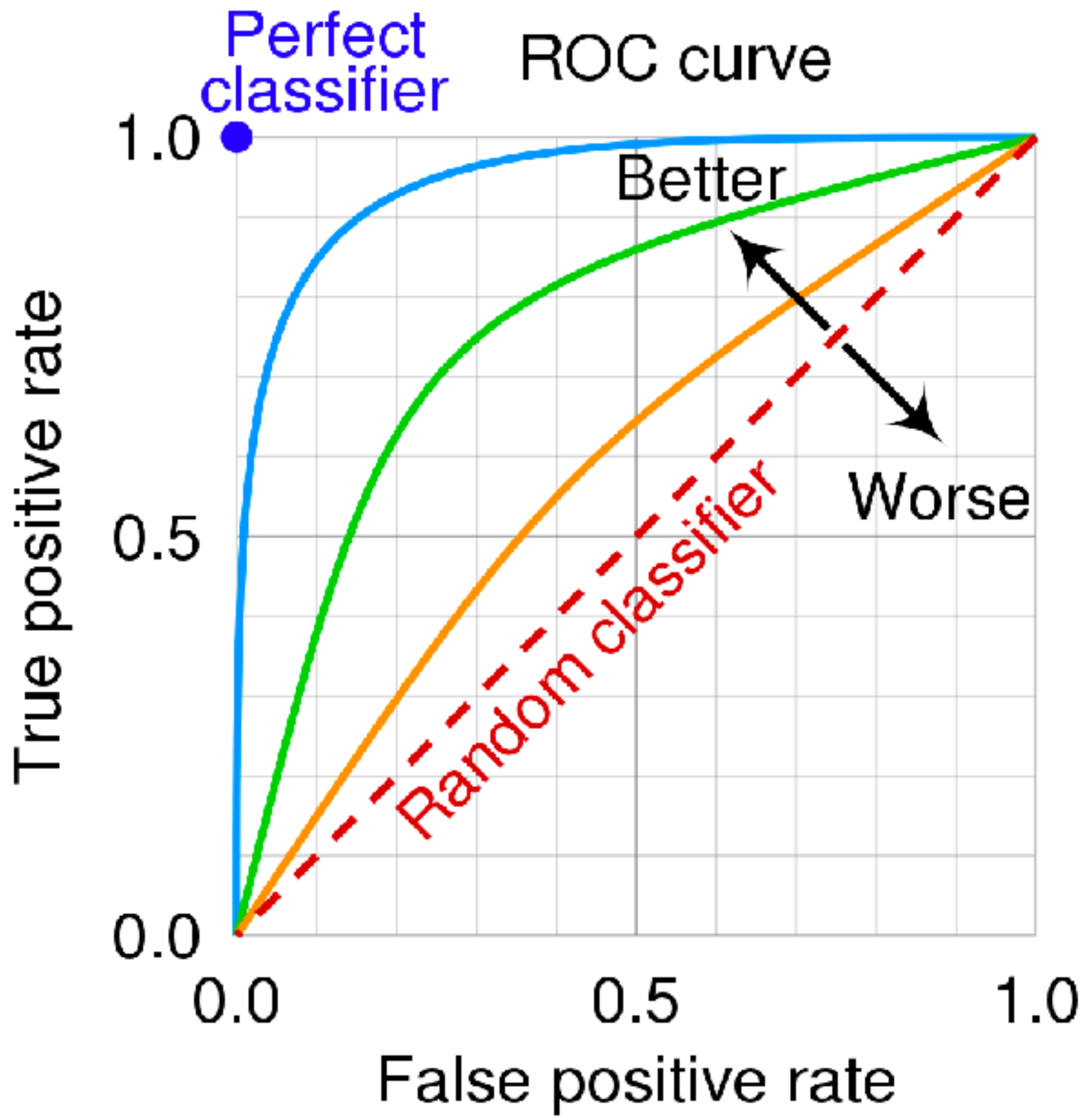
What have we estimated?

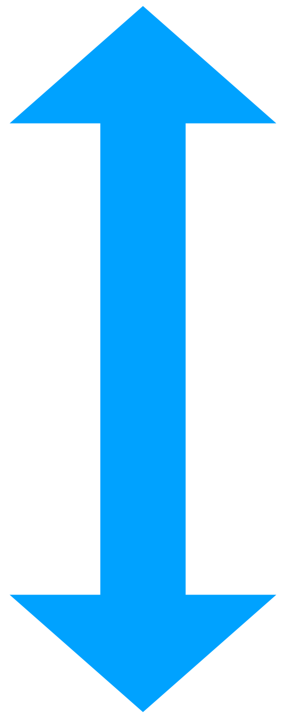
	$\hat{Y} = 1$	$\hat{Y} = 0$
$Y = 1$	TP	FN
$Y = 0$	FP	TN



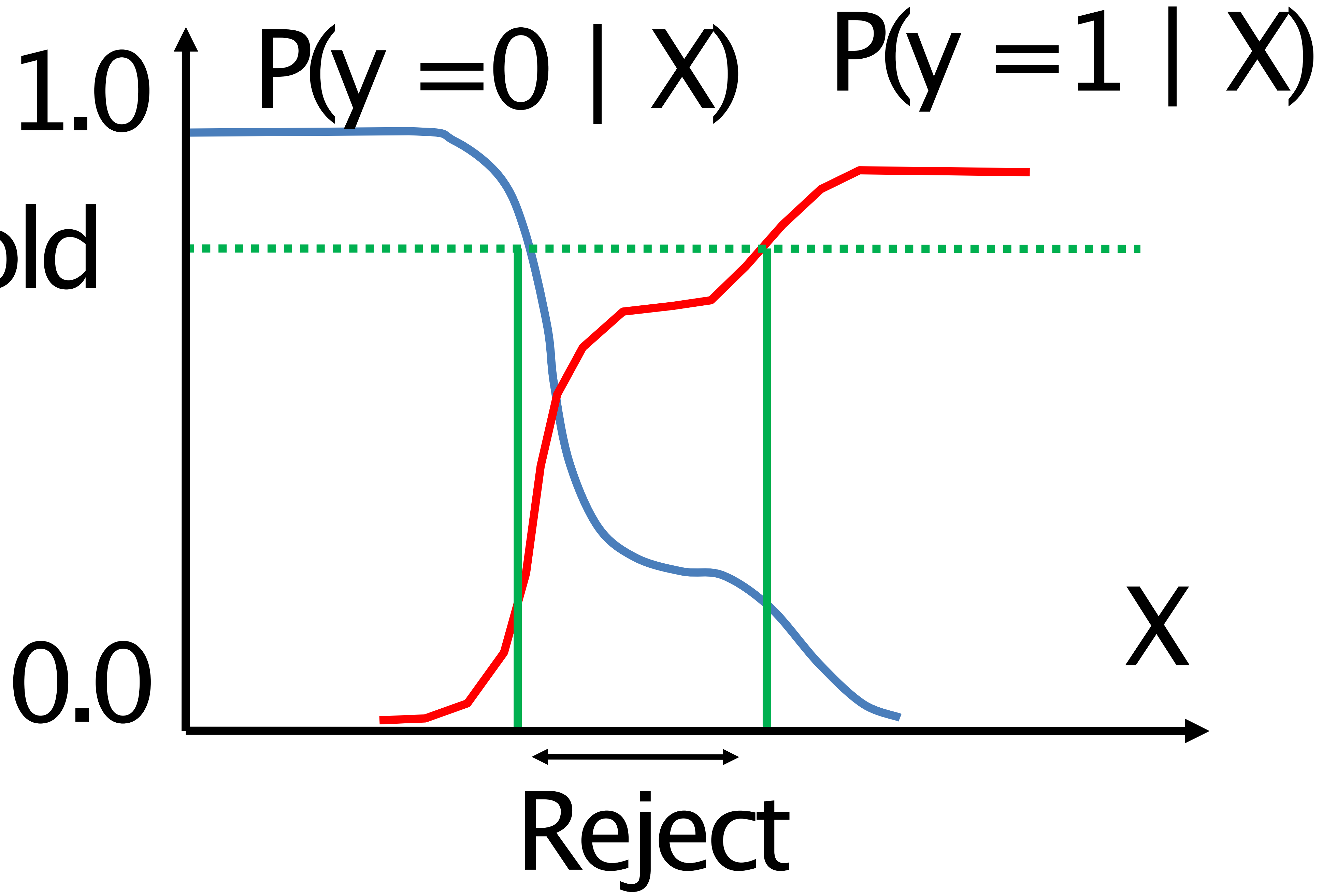
Murphy, Probabilistic Machine Learning

Can we tray different threshold levels?





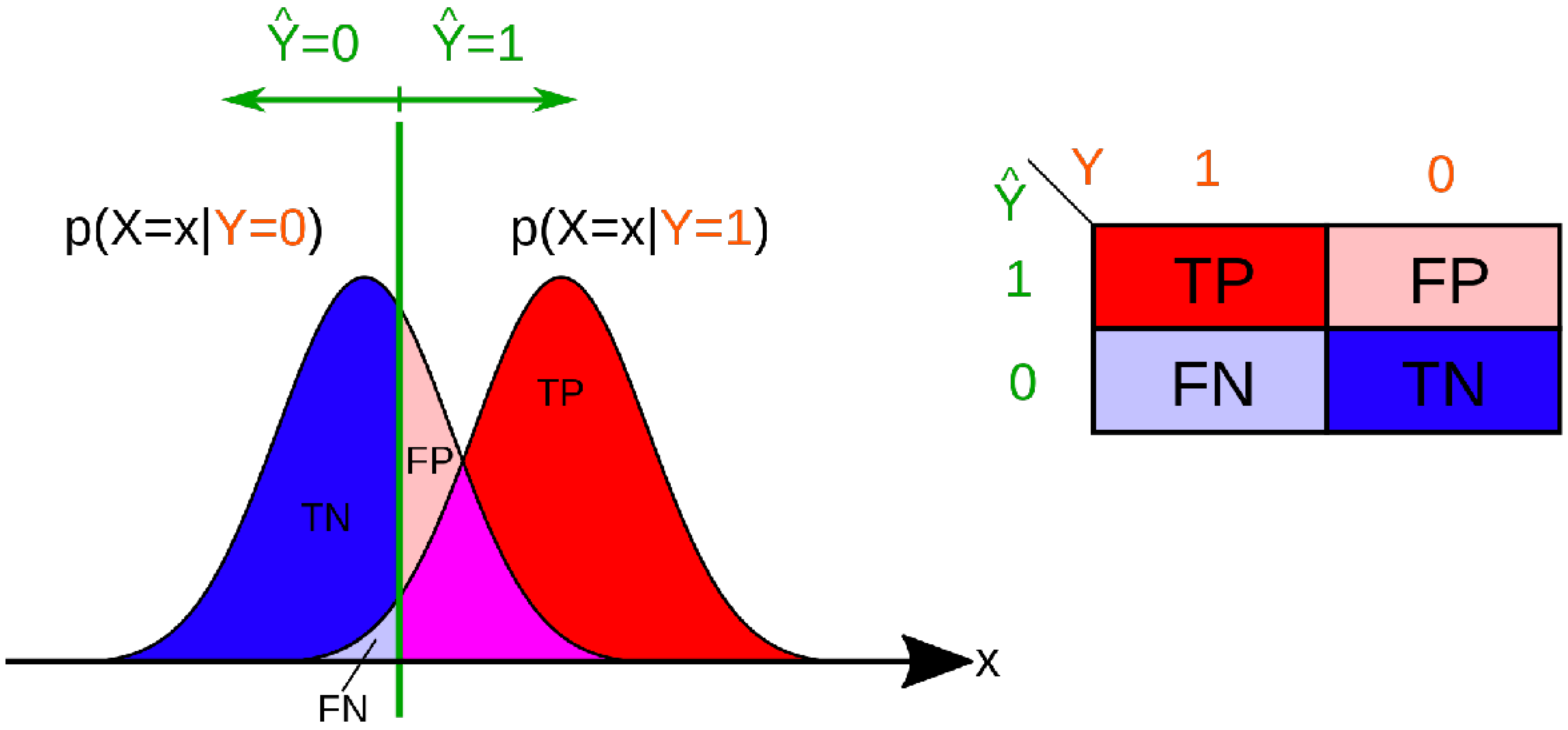
threshold



Murphy, Probabilistic Machine Learning

https://en.wikipedia.org/wiki/Receiver_operating_characteristic#/media/File:Roc_curve.svg

Receiver Operating Characteristic (ROC) curve



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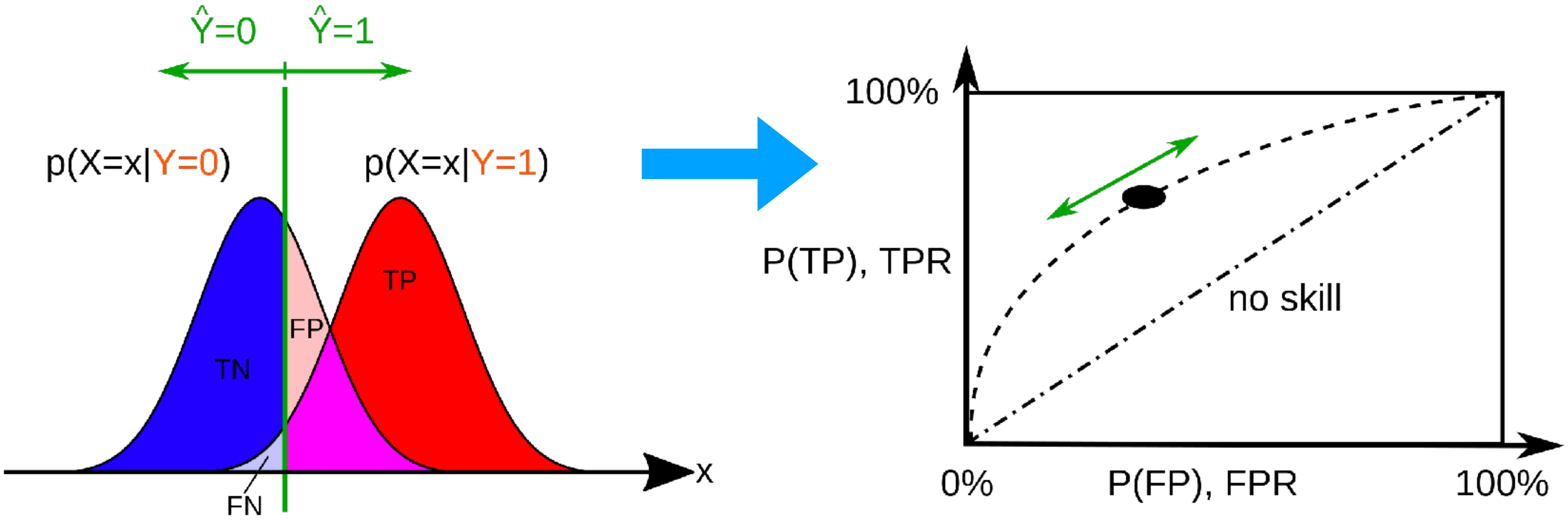
Draw ROC curve with different threshold levels



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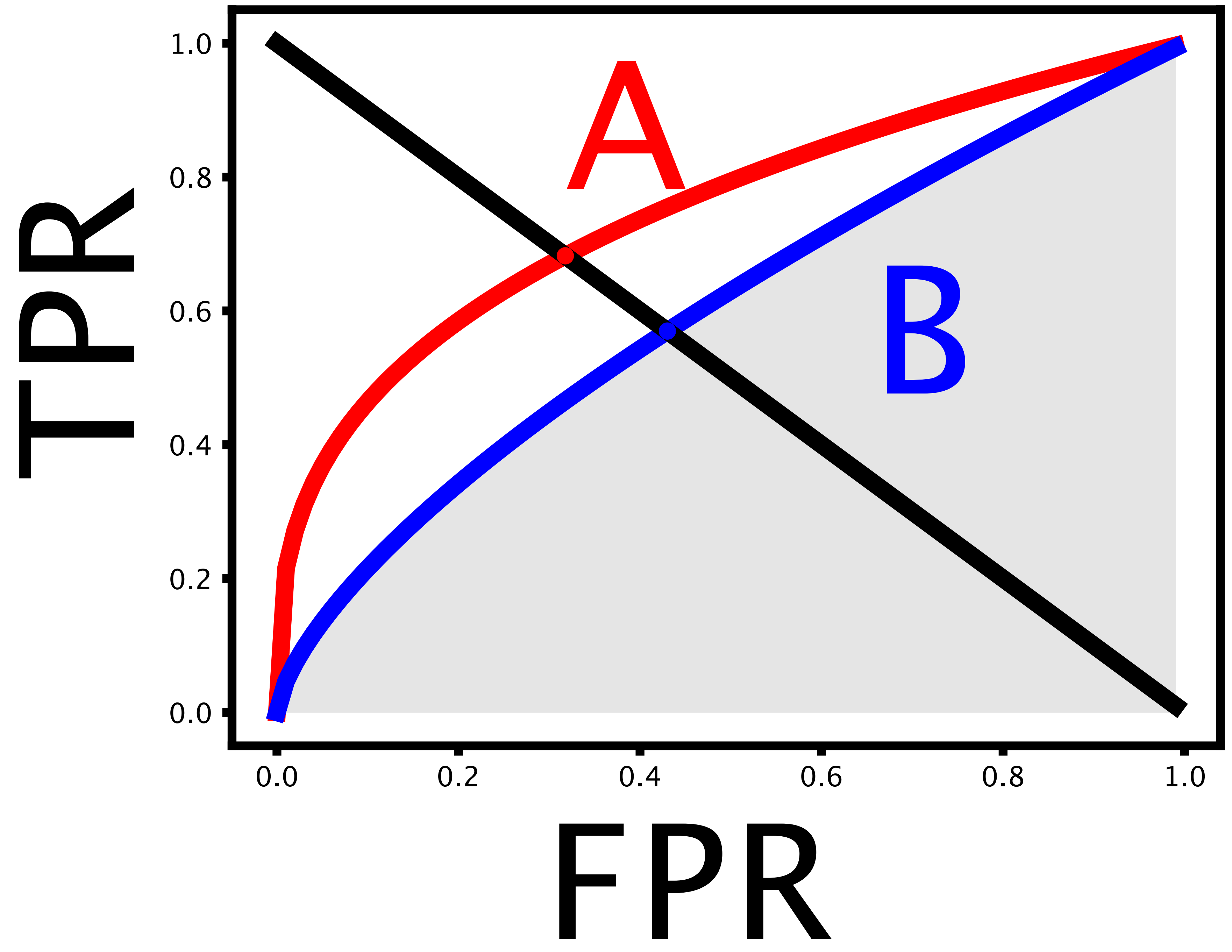
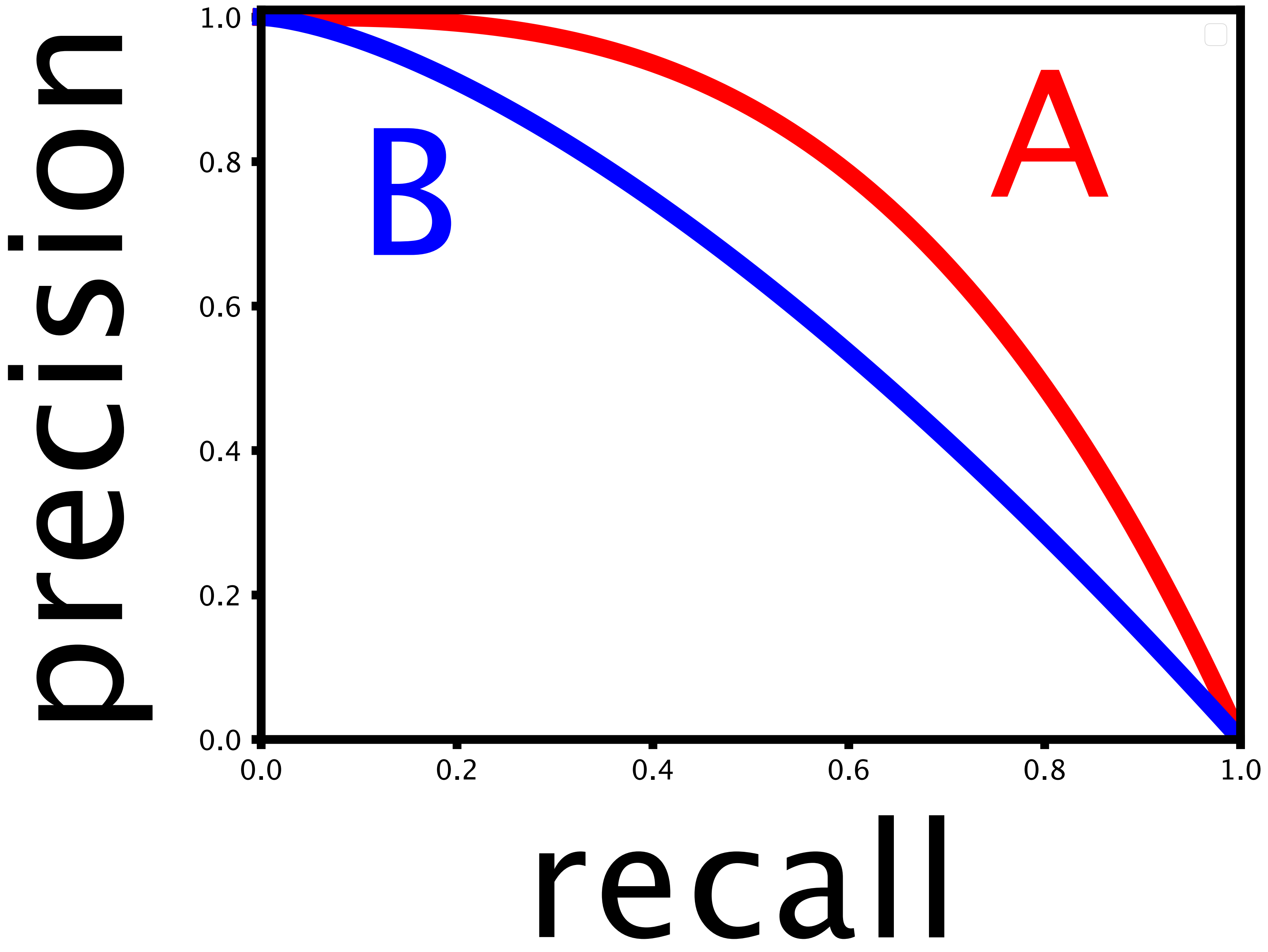
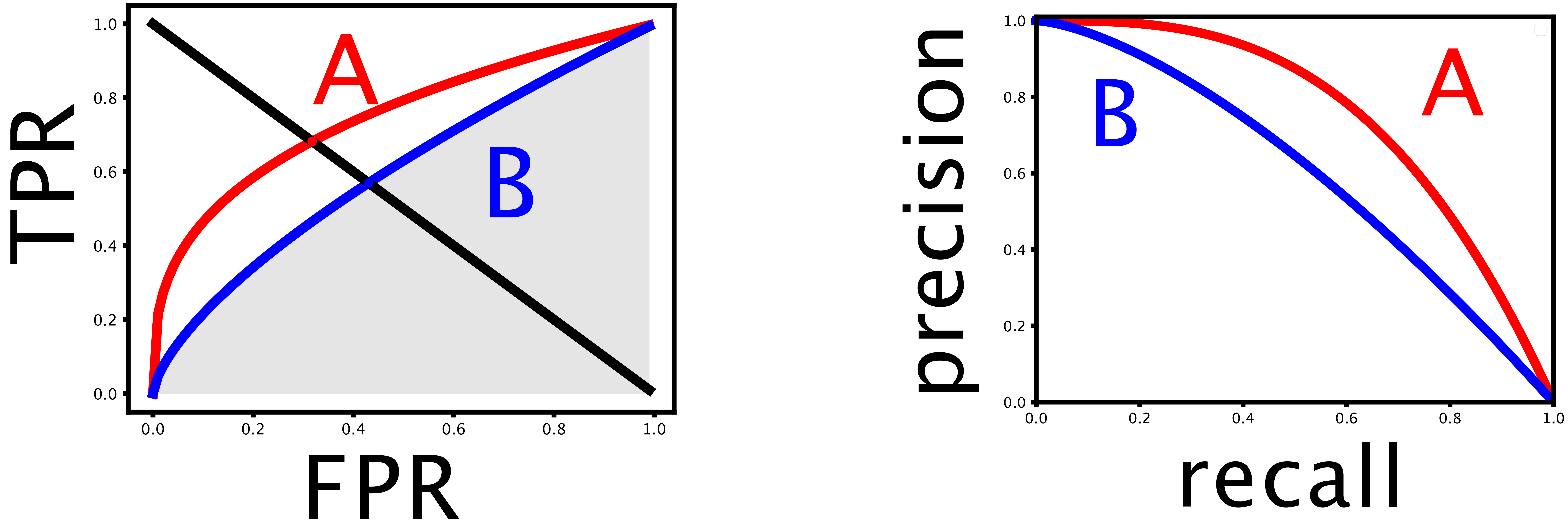
ROC and Precision Recall (PR) curves





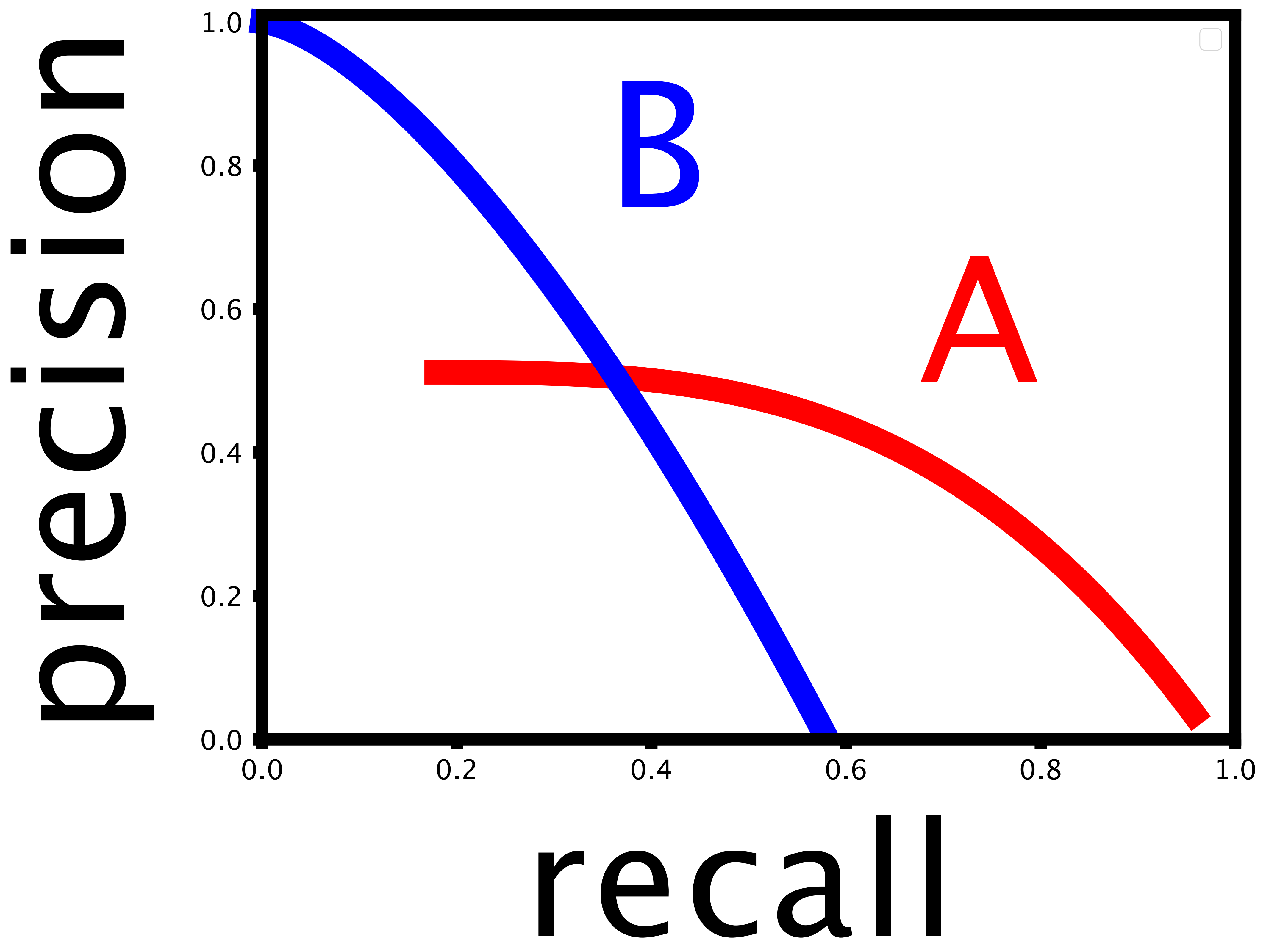
Murphy, Probabilistic Machine Learning

Which one to use?



Which method is better? A or B?

- In many genomics problems, we have so many cases to test
- How many mistakes (budget) can you afford until you cover X% of positive hits
- If we use this classifier in disease diagnosis, what will be more suitable?



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