Models as functions

10-701 Introduction to Machine Learning

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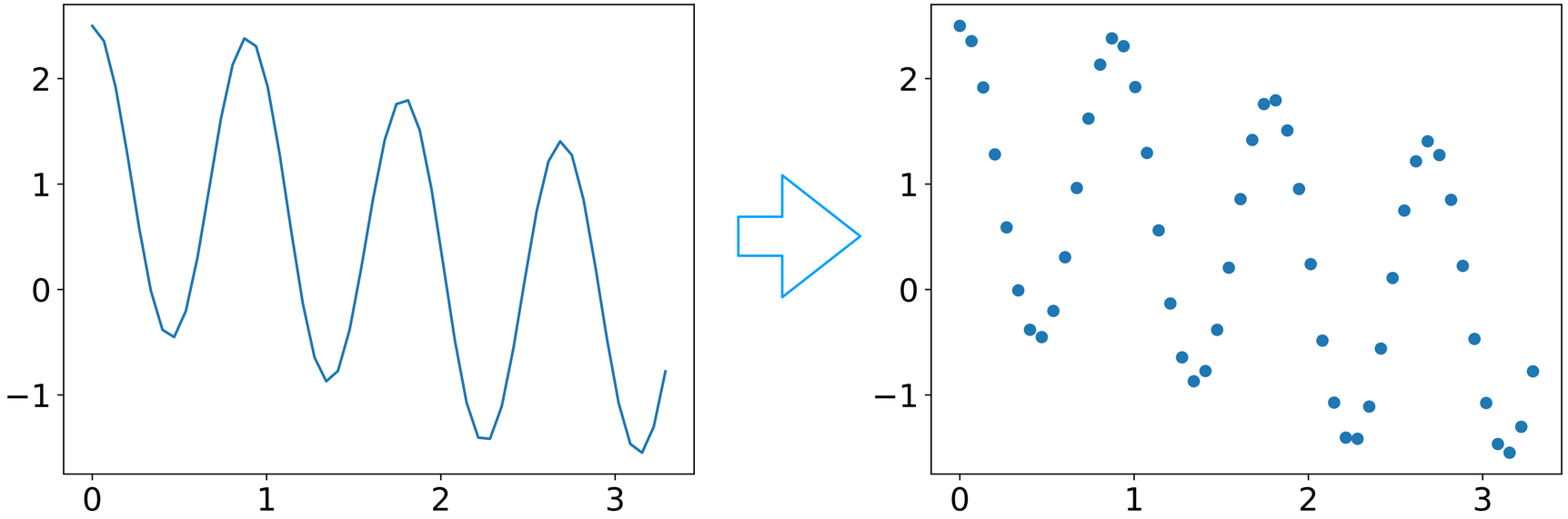
Models as functions

- Consider learning a model $y = f_\theta(x)$
- Can think of it two ways:
  - pick the best $\theta \in \Theta$ — e.g., run SGD on $L(\theta)$
  - pick the best $f \in \mathcal{F} = \{f_\theta \mid \theta \in \Theta\}$
    - never talk about θ
    - have to define $L(f)$
- Why?
  - parameter independence: if we define the same (or similar) $\mathcal{F}$ with different parameterizations, we get the same (or similar) behavior
  - understanding: θ isn't meaningful, f is what we care about

Functions are vectors



can help to think of f as if it were the sampled version — "components" are values $f(x)$, like components x_i of x, and "indices" are arguments x

- Just like we think of parameter space Θ as a subset of a vector space like $\mathbb{R}^d$, it helps to think of hypothesis space $\mathscr{F}$ as a subset of a vector space $\mathscr{H}$
  - each individual function f is a vector
  - i.e., satisfies the "vector space API": we can add $f + g$, scalar multiply $3f$, result is a vector

Vectors everywhere

- Defining a vector by its API is the ***coordinate-free*** or ***abstract*** view
- Lets us use our vector-manipulating skills in new places
- Other examples (that we won't use now):
  - matrices, tensors
  - differential operators: $\frac{d}{dx} + 3\frac{d}{dy}$
  - $\mathbb{Q}^d$ (with scalars from $\mathbb{Q}$), $\mathbb{R}^d$
  - polynomials
  - …

Staying sane: finite-dimensional version

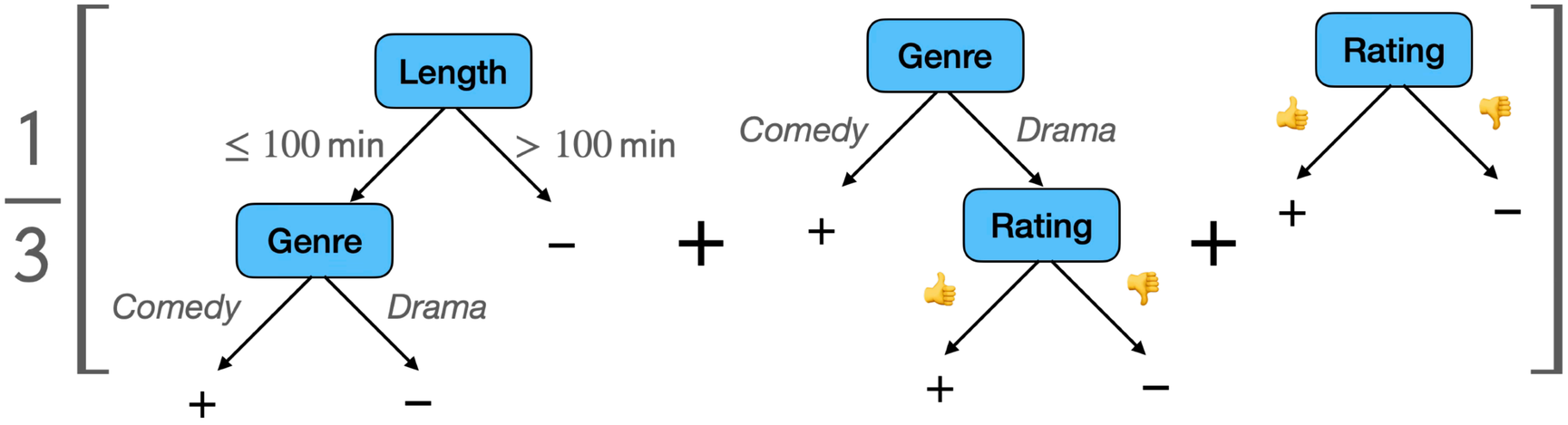
- Useful to connect back to old-fashioned linear-in-parameters functions $\mathcal{F} = \{f_\theta(x)\} = \{\theta \cdot \phi(x)\}$
  - parameter vector $\theta \in \mathbb{R}^d$
  - feature vector $\phi(x) \in \mathbb{R}^d$
  - feature function ϕ is fixed, may be nonlinear
  - but f_θ is linear in θ
- Won't get the full power of functional ML in this case, but it helps to understand what's going on

Storing a function

- Problem:
  - when we store a vector x, we do so by storing each component x_i
  - we can't afford to do this for the infinitely many components of f — its values $f(x)$
- Solution:
  - start from named functions like $\sin(x)$, e^x, or $T_i^d(x)$ — can even use $f_\theta(x)$, i.e., functions named by their parameters
  - construct other functions w/ vector space API:

    $$\sin(x) + 3e^x - 2T_1^5(x)$$ ← this is the ***span*** and original set is ***basis***
  - all such representations are finite: store as a list of coefficients × named fns
  - although long lists can get slow to work with!

Example of storing a complex function: bagging



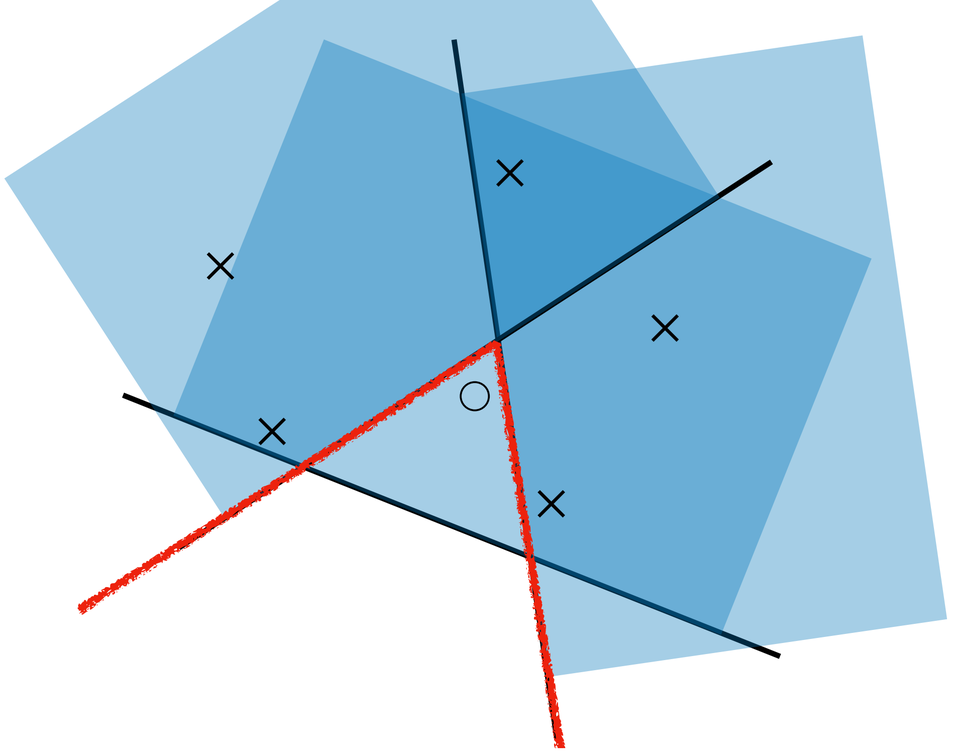
- We just saw an example: bagged classifier is stored as a sequence of vector-space operations on base learners like decision trees

Functional gradient

- What is the functions-as-vectors view good for?
- Example application: learning by ***functional gradient***
  - instead of gradient of loss wrt θ, take gradient wrt f — then step in function space r.t. parameter space
- Advantages:
  - convexity: with the extra flexibility of moving in function space, we avoid getting stuck in local optima
  - black-box access: someone has a fancy algorithm for fitting a function, but will only run it on their own servers
  - parameter independence: the answer doesn't change if we reparameterize our set of functions
- Todo: setup (choose $L(f)$), gradients (define $\nabla_f L$)
  - we'll use the example problem of learning a voted classifier for higher accuracy, called ***boosting***

Boosting

a wrapper we can put around any classification algorithm to try to make it stronger

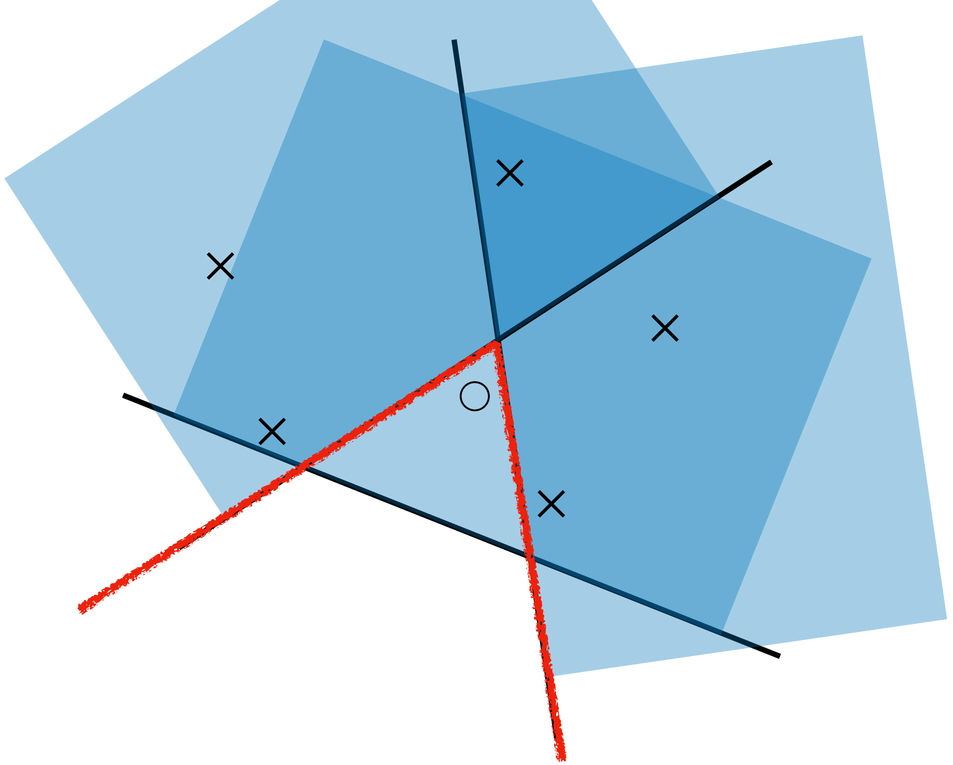


ex: vote of 3 linear classifiers

- Problem: learn a *voted classifier*
  - each base classifier $f_t : \mathbb{R}^d \to \{-1, 1\}$
  - vote: is $\sum_t f_t(x) \geq 0$?
    - or weighted vote: is $\sum_t \eta_t f_t(x) \geq 0$? (weights η_t)
  - wlog $\eta_t > 0$ for all t (assume $\mathcal{F}$ closed under negation)
  - normalize η_t if desired: divide by sum (doesn't affect vote)

can also do $\mathbb{R}^d \to [-1, 1]$ or even $\mathbb{R}^d \to \mathbb{R}$

Build a better classifier



ex: vote of 3 linear classifiers

- Voted classifier can be *strictly more expressive* than base classifiers: wedge-shaped red region $\notin \mathscr{F}$
- Take advantage of higher expressiveness to get higher accuracy ("boost" the base learner)
  - ***weak*** learner (base classifier, in $\mathscr{F}$) vs. ***strong*** learner (voted classifier, in $\mathscr{H}$)

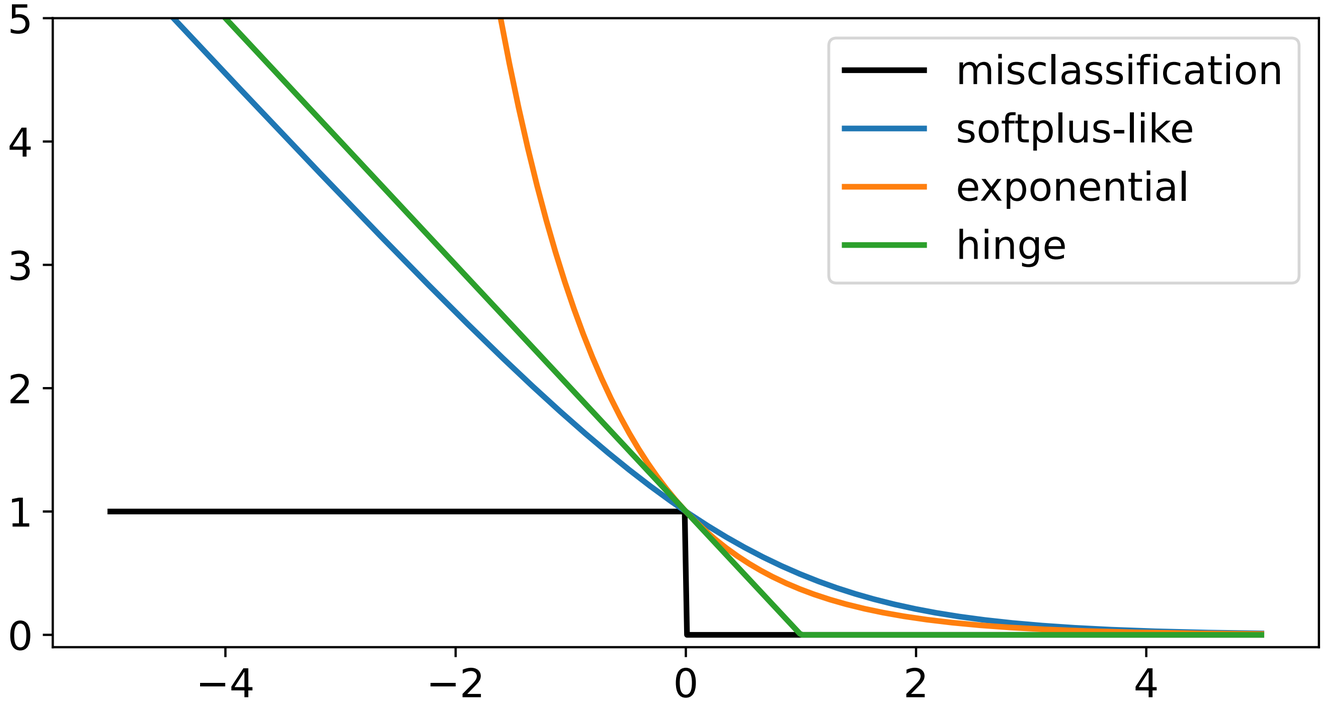
Comparison: boosting vs. bagging

- Both boosting and bagging are ensembles: vote over list of hypotheses from base hypothesis class
- But their purpose is different:
  - bagging tries to capture uncertainty (posterior over classifiers, predictive distribution) without necessarily beating the base hypothesis class
  - boosting tries to beat the base hypothesis class (weak learners), doesn't help much with estimating uncertainty
  - common boosting methods are focused on binary classification (though generalizations exist); bagging is easy to use for multi-class and regression

Comparison: boosting vs. bagging

- And their behavior is different
  - many small trees / weak hypotheses (boosting) vs. fewer large trees / stronger hypotheses (bagging)
  - fit different parts of target concept (boosting) vs. all of it in different ways (bagging)
  - limits overfitting by max margin (boosting) vs. by randomization and averaging (bagging)

Boosting setup



- Given a training set $\{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$ where
  - $x^{(i)} \in \mathcal{X}$ (any feature set)
  - $y^{(i)} \in \{\pm 1\}$ (binary classification, classes +1 and –1)

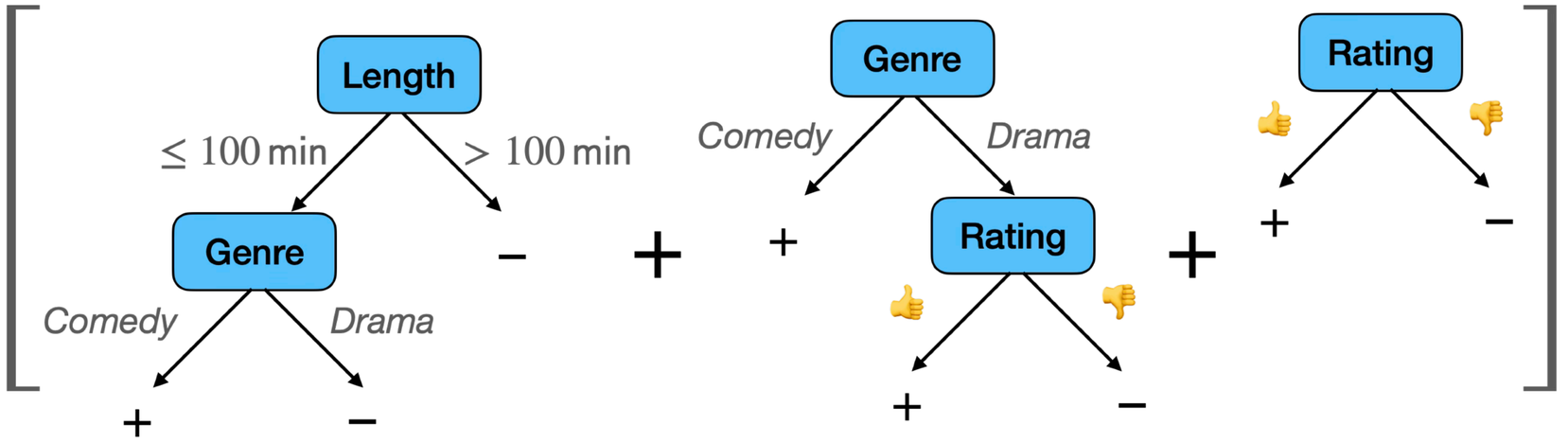
  and a base hypothesis set $\mathcal{F} \subset \mathcal{X} \to \{\pm 1\}$
- Pick a convex per-example loss function ℓ that upper-bounds misclassification loss

minimizing ℓ means we want its argument to be positive

we'll use ℓ to construct total loss L

Boosting loss

$$\mathcal{H} = \{ \sum_t \eta_t f_t \mid f_t \in \mathcal{F} \}$$



$y^{(i)} f(x^{(i)})$: want $f(x^{(i)}) > 0$ when $y^{(i)} = +1$,
$f(x^{(i)}) < 0$ when $y^{(i)} = -1$

- Our goal:

$$\min_{f \in \mathcal{H}} L(f) = \sum_{i=1}^{N} \ell(y^{(i)} f(x^{(i)}))$$

  - where $\mathcal{H}$ = weighted votes over elements of $\mathcal{F}$ (before thresholding, unnormalized weights)
- Minimize a convex loss function over a convex set

Finite-d analogy

$$\min_{f \in \mathcal{H}} L(f) = \sum_{i=1}^{N} \ell(y^{(i)} f(x^{(i)}))$$

- If our base learners are linear-in-parameters functions, then $\mathcal{F} = \mathcal{H} = \mathbb{R}^d$: $\sum_t \eta_t(\phi(x) \cdot \theta_t) = \phi(x) \cdot \sum_t \eta_t \theta_t$
  - i.e., we were already convex, so boosting doesn't increase expressiveness

note: outputs are in $\mathbb{R}$ not $\{\pm 1\}$ but this is OK

- So the optimization becomes

$$\min_{\theta \in \mathbb{R}^d} \sum_{i=1}^{N} \ell(y^{(i)} \phi(x^{(i)}) \cdot \theta)$$

- This setup is exactly what we used for linear classifiers:
  - $\ell(z) = \ln(1 + \exp(-z))$ yields logistic regression
  - $\ell(z) = [-z]_+$ yields perceptron
- So, novelty of boosting is handling ∞-dim nonconvex $\mathcal{F}$

Gradient of loss

$$\min_{f \in \mathcal{H}} L(f) = \sum_{i=1}^{N} \ell(y^{(i)} f(x^{(i)}))$$

- Functional gradient descent update: subtract a multiple of $\nabla_f L(f)$ from current hypothesis f
- Still need to define ∇_f but let's see what we can do given that it will act like other derivative operators:

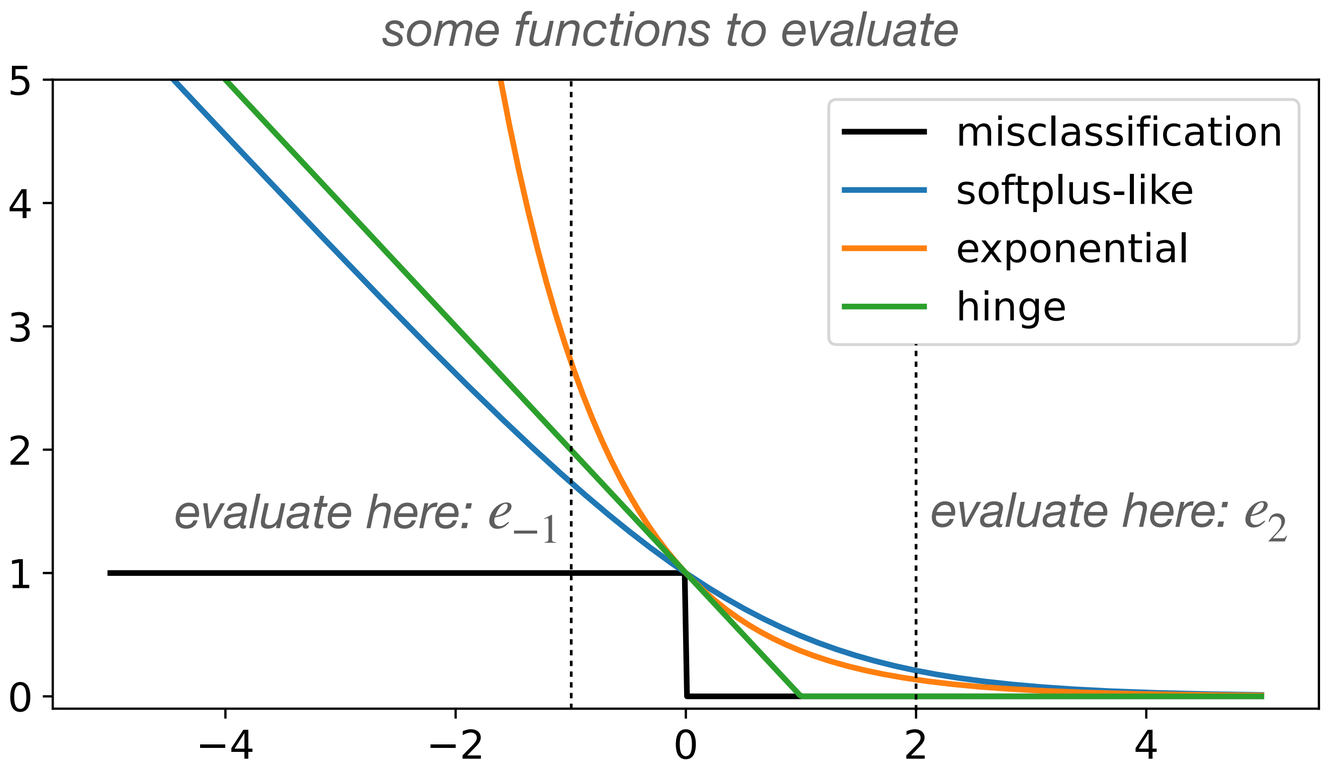
$$\begin{aligned} \nabla_f L(f) &= \sum_{i=1}^{N} \nabla_f \ell(y^{(i)} f(x^{(i)})) \\ &= \sum_{i=1}^{N} \ell'(y^{(i)} f(x^{(i)}))\, y^{(i)}\, \nabla_f f(x^{(i)}) \end{aligned}$$

- So, just need to figure out what to do with $\nabla_f f(x^{(i)})$

Functionals

- What is the data type of $\nabla_f f(x)$?
- Recall: derivatives represent linear functions
  - e.g., $d\|x\|^2 = 2x^\top dx$: the change in $\|x\|^2$ is locally approximated by a linear function of the change in x
- So we want a function that maps $df \in \mathscr{H}$ (the change in f) to $d(f(x)) \in \mathbb{R}$ (the change in $f(x)$)
- This is called a ***functional***:
  - a function that takes another function as its argument and returns a scalar
  - in our case a linear functional of type $\mathscr{H} \to \mathbb{R}$
- Other examples: $L(f)$ is a (nonlinear) functional, and…

Ex: point evaluation functional



- ***Point evaluation*** functional e_x is defined as $e_x(f) = f(x)$
- E.g., $e_2(\text{hinge}) = 0$ or $e_{-1}(\text{exponential}) = 2.718$
- e_x is a linear functional:

$$e_2(3 \sin x + 1) = 3e_2(\sin x) + e_2(1) = 3 \sin 2 + 1$$

Linear functionals as inner products

- We've encountered some useful examples of linear functionals: $\nabla_f f(x)$ and e_x
- In $\mathbb{R}^d$ we can always write a linear functional $a(x)$ as $\tilde{a} \cdot x$ for some vector $\tilde{a}$ (the ***representer*** of $a(x)$)
  - in fact we often don't bother distinguishing: use a for both and let context decide whether we mean a vector $a \in \mathbb{R}^d$ or a linear functional $a \in \mathbb{R}^d \to \mathbb{R}$
- This property is essential for gradient descent (so essential we rarely even think about the type cast):
  - each step adds a gradient (a linear functional) to the parameter we're trying to optimize (a vector)
  - if they were incompatible types, addition would break
- So for functional gradient, we need to define an inner product and interpret $\nabla_f f(x)$ as $\langle g, df \rangle$ for some g

Inner product

- A valid inner product $\langle f, g \rangle$ satisfies:
  - ***linear*** in each argument: $\langle 3f + g, h \rangle = 3\langle f, h \rangle + \langle g, h \rangle$
  - ***symmetric***: $\langle f, g \rangle = \langle g, f \rangle$
  - ***positive definite***: $\langle f, f \rangle = 0$ iff f is the all-zero function
- It tells us which pairs of unit vectors are similar (high inner product) or different (low or negative inner product)
- Typically $\exists$ many ways to define an inner product on a set of functions, leading to spaces that behave differently
  - e.g., $\langle f, g \rangle = \int_x f(x)g(x)\,dx$ (like dot, leads to L_2)
  - or $\langle f, g \rangle = \frac{1}{2}\int_x f(x)g(x)\,dx + \frac{1}{2}\int_x f'(x)g'(x)\,dx$ (leads to a Sobolev space) — a good example to keep in mind, since L_2 fns are too non-smooth to be good for ML
  - or (many) other examples we'll define later

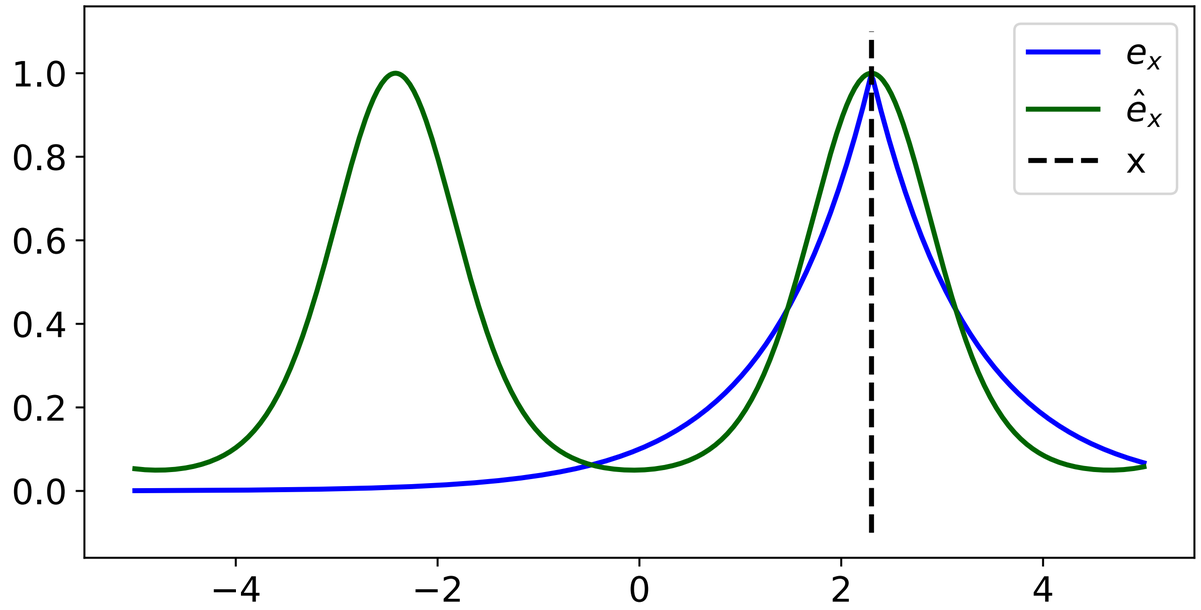
Finite-d analogy

- For linear-in-parameters functions,
  - the inner product is the usual dot product on $\mathbb{R}^d$
  - the representer of $f_\theta(x) = \theta \cdot \phi(x)$ is the vector θ
  - the representer of a point-evaluation functional is $e_x = \phi(x)$
- So, to evaluate a function at a point, we take the dot product between f_θ's vector θ and e_x's vector $\phi(x)$:
  - $e_x(f_\theta) = \langle e_x, f_\theta \rangle = \phi(x) \cdot \theta$
- Surprising conclusion: point-evaluation functionals are the generalization of ***feature vectors*** of points

Point-eval functionals as feature vectors

point-evaluation functionals are related to kernels — more about this soon

two different point evaluation functionals for the same x, different inner products



blue is for Sobolev space defined above

- We'll shortly assume the representer e_x for a point evaluation functional exists and is a function in $\mathscr{H}$ — i.e., we can evaluate it at other values x'
- The shape of e_x depends on how we define inner product (which pairs of unit vectors in $\mathscr{H}$ we think are similar)
- The function values $(e_x(3.27), e_x(-1.05), \ldots)$ act like features of the point x: high for x' we consider similar to x

Extending the API

- We've just extended our API
  - from vector space (supports addition and scalar product)
  - to ***inner product space*** (also supports $\langle f, g \rangle$)
- Turns out we need a couple more operations before we can define gradients:
  - taking limit of a sequence $\lim_{t\to\infty} f_t = f$: adding limits to our API yields a ***Hilbert space***
  - representer for point evaluation, $x \mapsto e_x$ (type $\mathcal{X} \to \mathcal{H}$): yields a ***reproducing kernel Hilbert space*** or ***RKHS***
- All these ops work fine on $\mathbb{R}^d$, so adding them to API lets us treat functions even more like ordinary vectors

Gradients

- New API lets us define and compute derivative $\nabla_f f(x)$
- We added three things: inner product, limits, point eval
  - inner product lets us express derivative as a vector $g \in \mathcal{H}$ representing the linear functional $\langle g, df \rangle$
  - limits let us define which g we want:

    if $df \to 0$ then $\dfrac{\|[(f + df)(x) - f(x)] - \langle g, df \rangle\|}{\|df\|} \to 0$
  - we'll shortly see that $x \mapsto e_x$ ensures gradient exists and lets us compute it

Gradients

- In fact it turns out ***the derivative*** $\nabla_f f(x)$ ***is exactly*** e_x
  - to see why: $(f + df)(x) = f(x) + (df)(x)$
  - so the change in $f(x)$ is df evaluated at x, or $\langle e_x, df \rangle$
- Assuming the API operation $x \mapsto e_x$ means assuming that e_x must exist in $\mathscr{H}$
  - i.e., the assumption restricts how we choose an inner product in order to guarantee $f(x)$ is differentiable wrt f

Good-enough step direction

- Substituting in, the gradient we want is

$$\nabla_f L(f) = g = \sum_{i=1}^{N} \ell'(y^{(i)} f(x^{(i)}))\, y^{(i)} e_{x^{(i)}}$$

- Problem: this g probably isn't in $\mathcal{F}$
- So we have to work with it as a list (slow) instead of as a base classifier (fast)
- Solution: instead of using gradient g directly, pick an element of $\mathcal{F}$ that has *positive inner product* with desired step direction $-g$
  - recall that gradient descent still works if we use an approximate step, as long as on average the inner product between step and $-g$ is enough bigger than 0

Solving for the step direction

to ensure inner product is big enough, we can (approximately) maximize

$$f_t = \max_{f \in \mathcal{F}} \langle f, -g \rangle$$

$$= \max_{f \in \mathcal{F}} \langle f, \; -\sum_{i=1}^{N} \ell'(y^{(i)} f(x^{(i)}))\, y^{(i)} e_{x^{(i)}} \rangle$$

$$= \max_{f \in \mathcal{F}} \sum_{i=1}^{N} -\ell'(y^{(i)} f(x^{(i)}))\, y^{(i)} \langle f, e_{x^{(i)}} \rangle$$

$$= \max_{f \in \mathcal{F}} \sum_{i=1}^{N} \underbrace{\alpha^{(i)}}_{\text{weight}} \underbrace{y^{(i)} f(x^{(i)})}_{\substack{+1 \text{ if correct} \\ -1 \text{ if error}}}$$

ℓ' is negative, so $\alpha^{(i)} > 0$

- Maximize weighted number of correct predictions: a classification problem on weighted copy of our dataset!
- More weight for points whose current signed prediction $z^{(i)} = y^{(i)} f(x^{(i)})$ has big effect on loss (big derivative ℓ')

Boosting summary

- For $t = 1,2,\ldots$:
  - compute weights $\alpha_t^{(i)}$ for each point: $\alpha_1^{(i)}$ uniform, $\alpha_t^{(i)}$ based on influence of point i on loss at step $t-1$
  - find a good weak learner f_t (an approximate functional gradient): correlation $> \varepsilon$ on weighted data
  - take a step in direction f_t: add f_t to our vote, weight η_t
- Different choices of ℓ and η_t yield different boosting methods

Did this help?

- In order to solve our classification problem, we have to repeatedly reweight our data and solve a classification problem

Did this help?

- In order to solve our ***strong*** classification problem, we have to repeatedly reweight our data and solve a ***weak*** classification problem

Did this help?

- In order to solve our ***strong*** classification problem, we have to repeatedly reweight our data and solve a ***weak*** classification problem

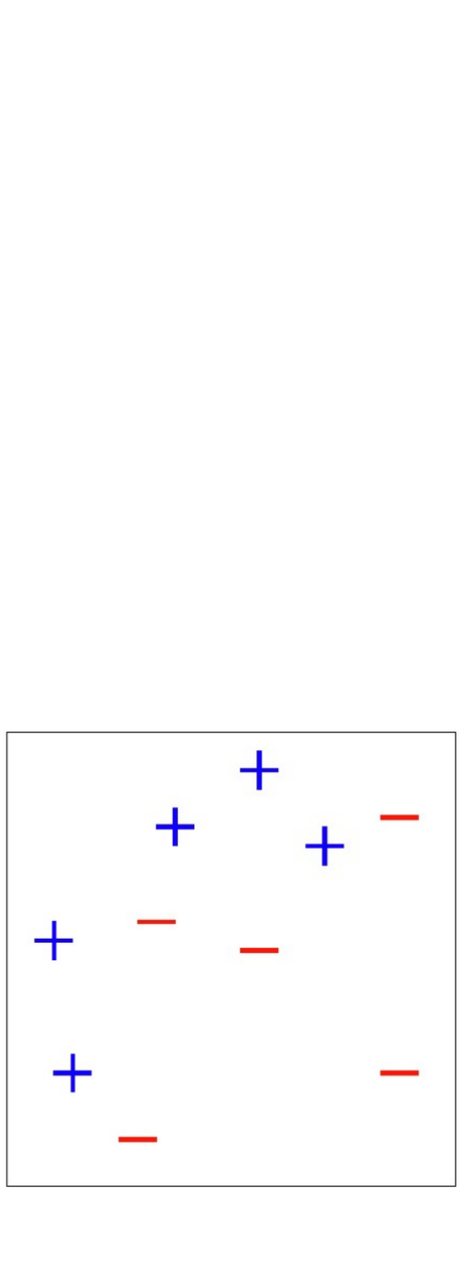
- Idea: if base algorithm (the weak learner) can keep doing just a bit better than chance, then final boosted classifier (the strong learner) can keep improving
  - eventually will get zero error on the training set

AdaBoost

uses exponential loss e^{-z}

- Input: number of rounds T, dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$
- Initialize datapoint weights $\alpha_0^{(i)} = \frac{1}{N}$ for all i
- For $t = 1, \ldots, T$:
  - Train a weak learner f_t by minimizing *weighted* training error on $\mathcal{D}$ (weights $\alpha_{t-1}^{(i)}$)
  - Find weighted training error of f_t: $\varepsilon_t = \sum_{i=1}^{N} \alpha_{t-1}^{(i)} \mathbb{I}(y^{(i)} \neq f_t(\mathbf{x}^{(i)}))$
  - Compute the vote weight of f_t: $\eta_t = \frac{1}{2} \ln \frac{1 - \varepsilon_t}{\varepsilon_t}$
  - Update datapoint weights: $\alpha_t^{(i)} = \frac{\alpha_{t-1}^{(i)}}{Z_t} \cdot \begin{cases} e^{-\eta_t} & y^{(i)} = f_t(\mathbf{x}^{(i)}) \\ e^{\eta_t} & \text{o/w} \end{cases}$ (Z_t is normalizer)
- Return: weighted vote classifier $\hat{y} = \text{sign}\left(\sum_{t=1}^{T} \eta_t f_t(\mathbf{x}) \right)$

AdaBoost example



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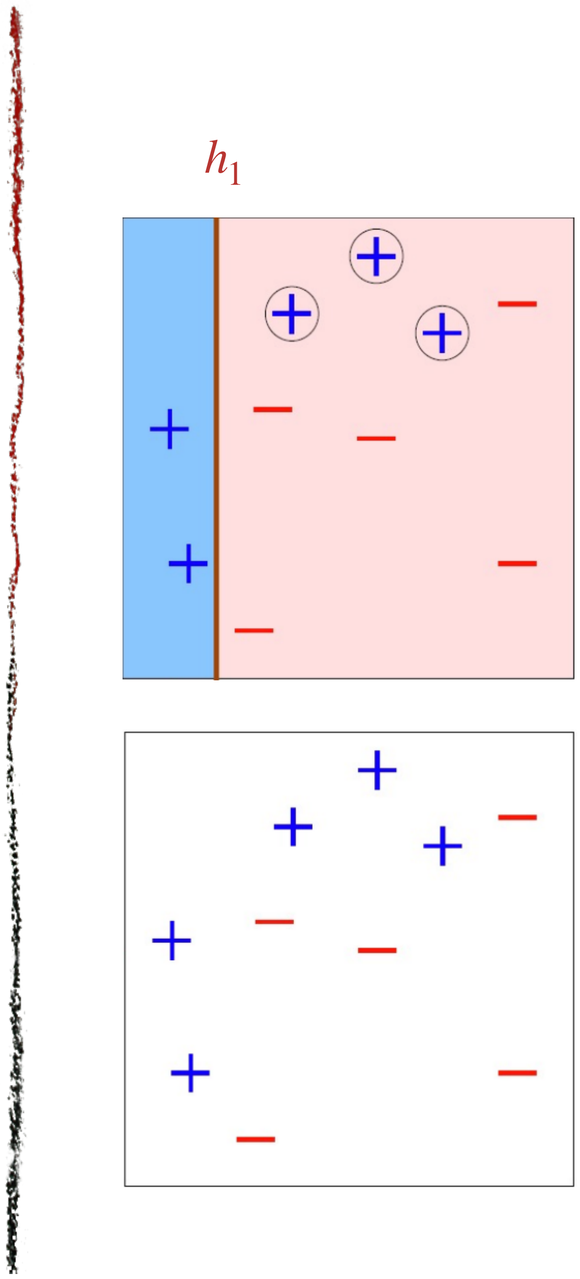
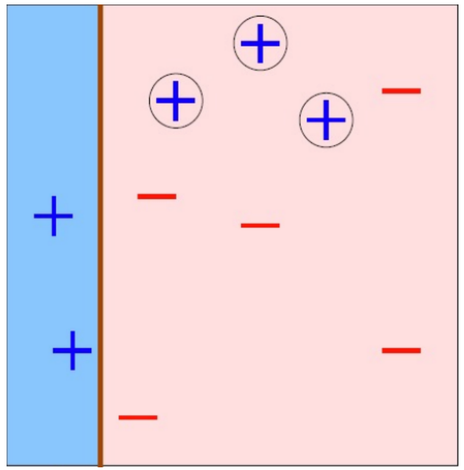


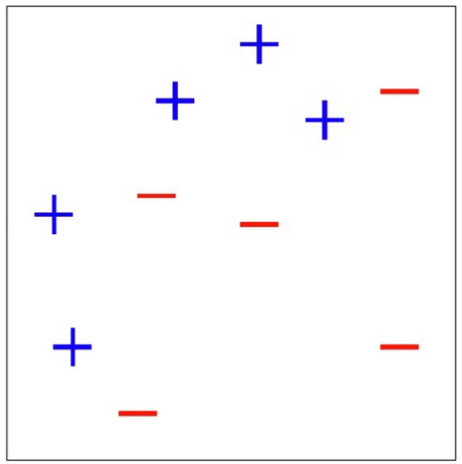
AdaBoost example

$\epsilon_1 = 0.3$

$\alpha_1 = 0.42$

h_1





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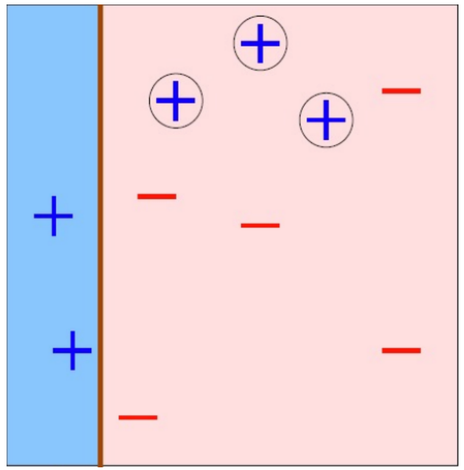
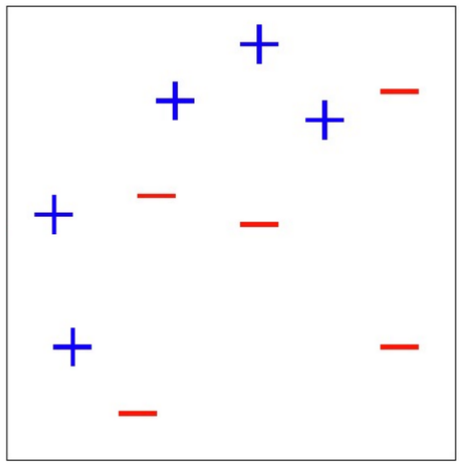
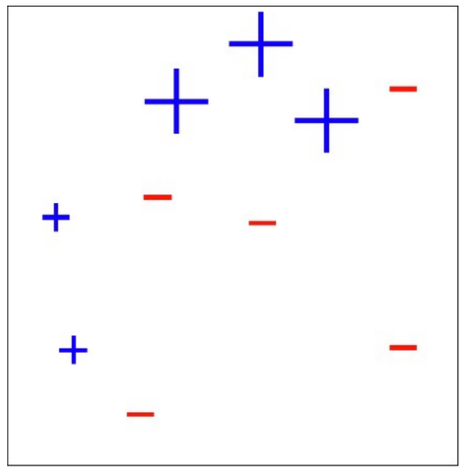


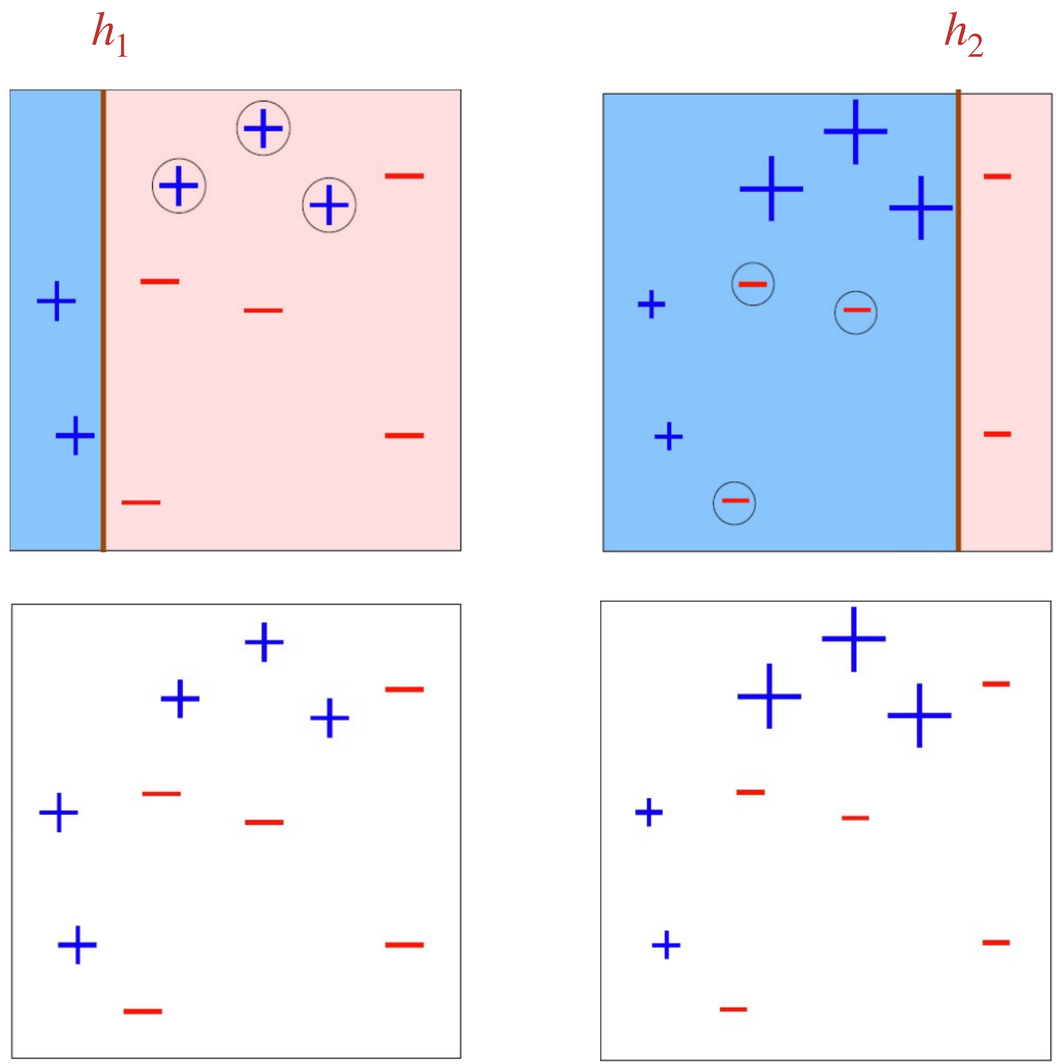




AdaBoost example

$\epsilon_1 = 0.3$

$\alpha_1 = 0.42$



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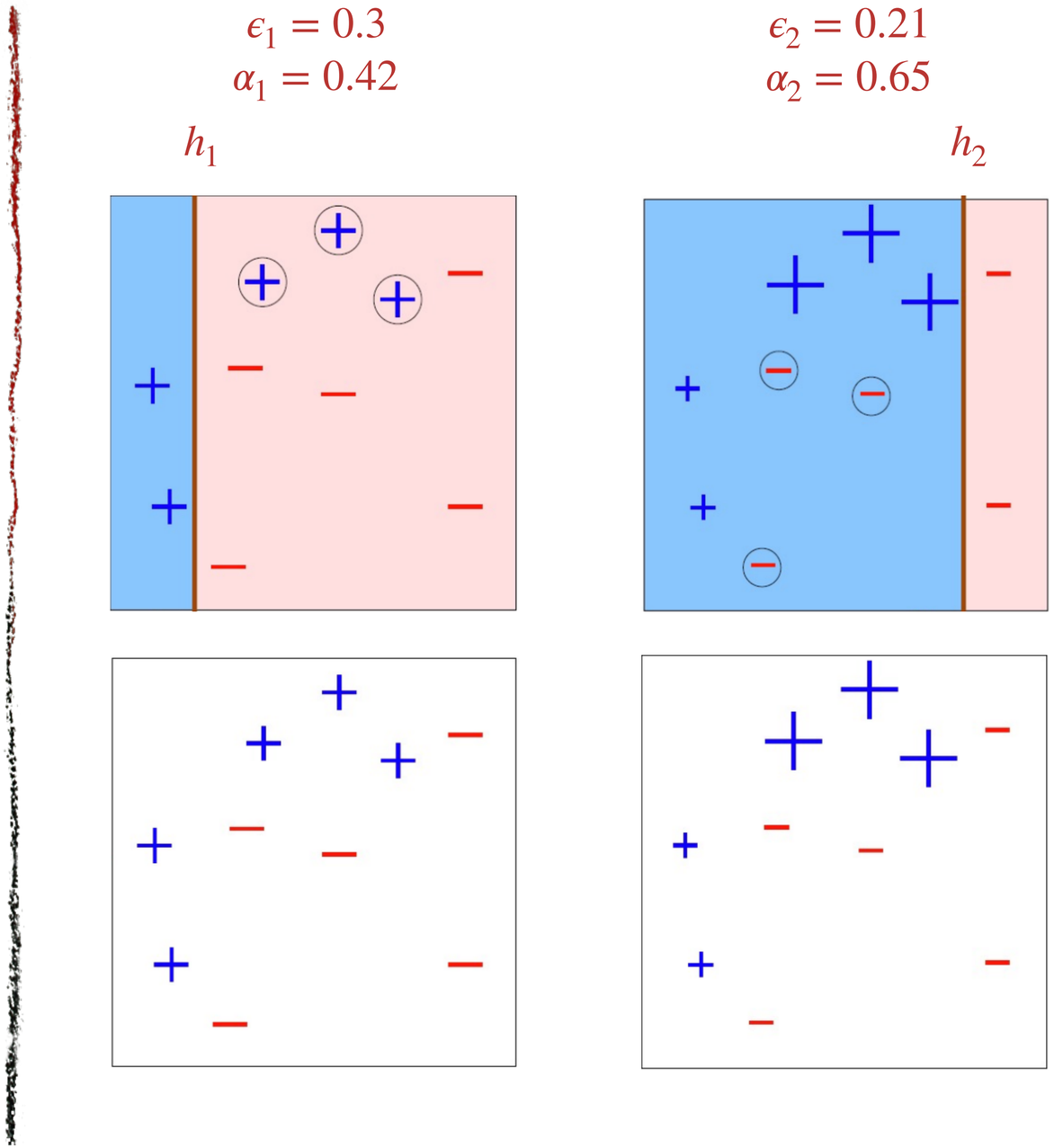
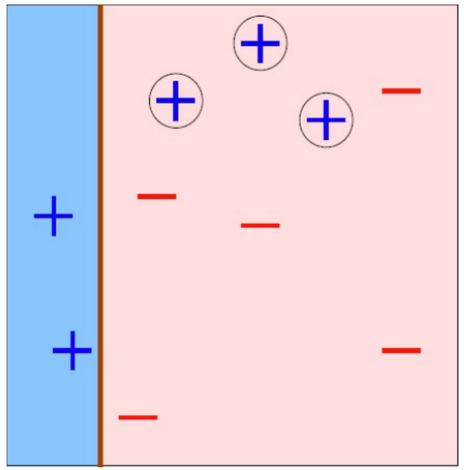
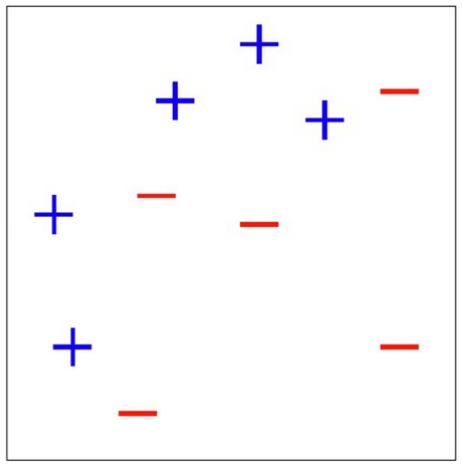


AdaBoost example

$\epsilon_1 = 0.3$
$\alpha_1 = 0.42$

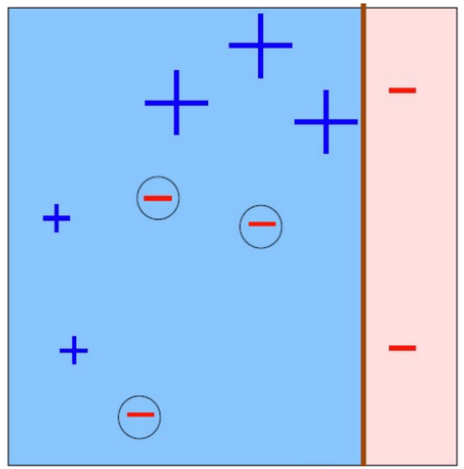
h_1

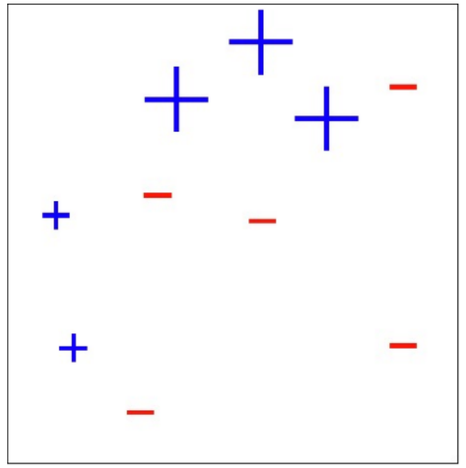




$\epsilon_2 = 0.21$
$\alpha_2 = 0.65$

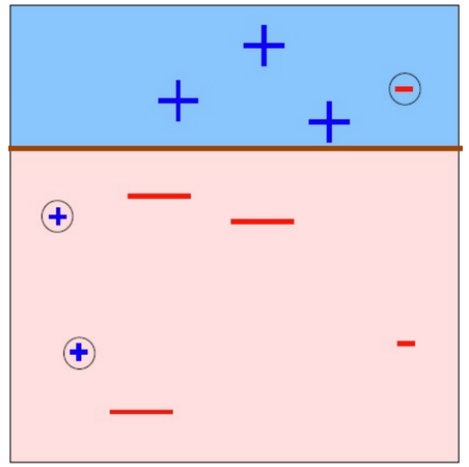
h_2

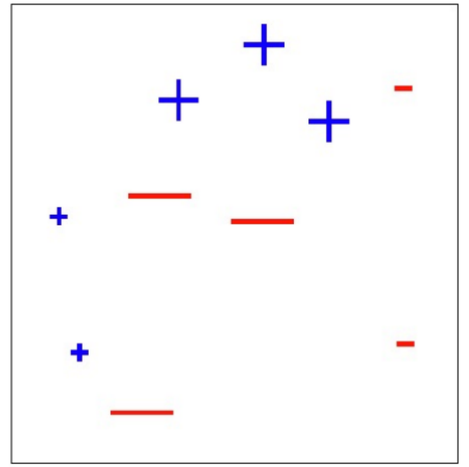




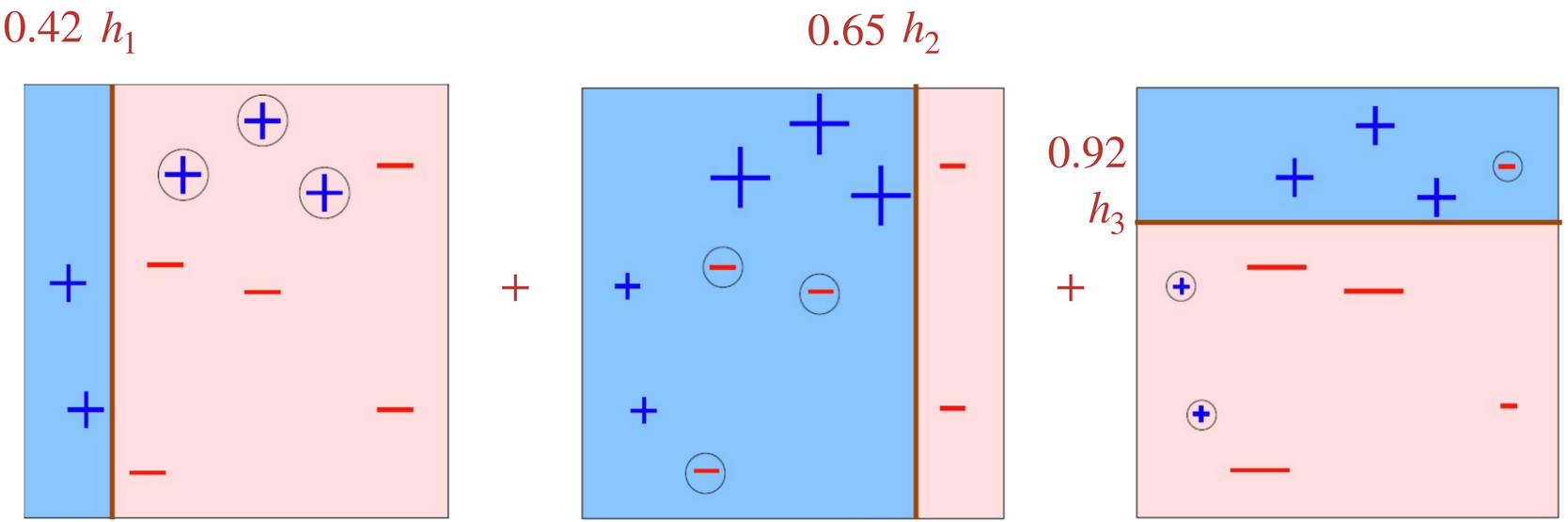
$\epsilon_3 = 0.14$
$\alpha_3 = 0.92$

h_3

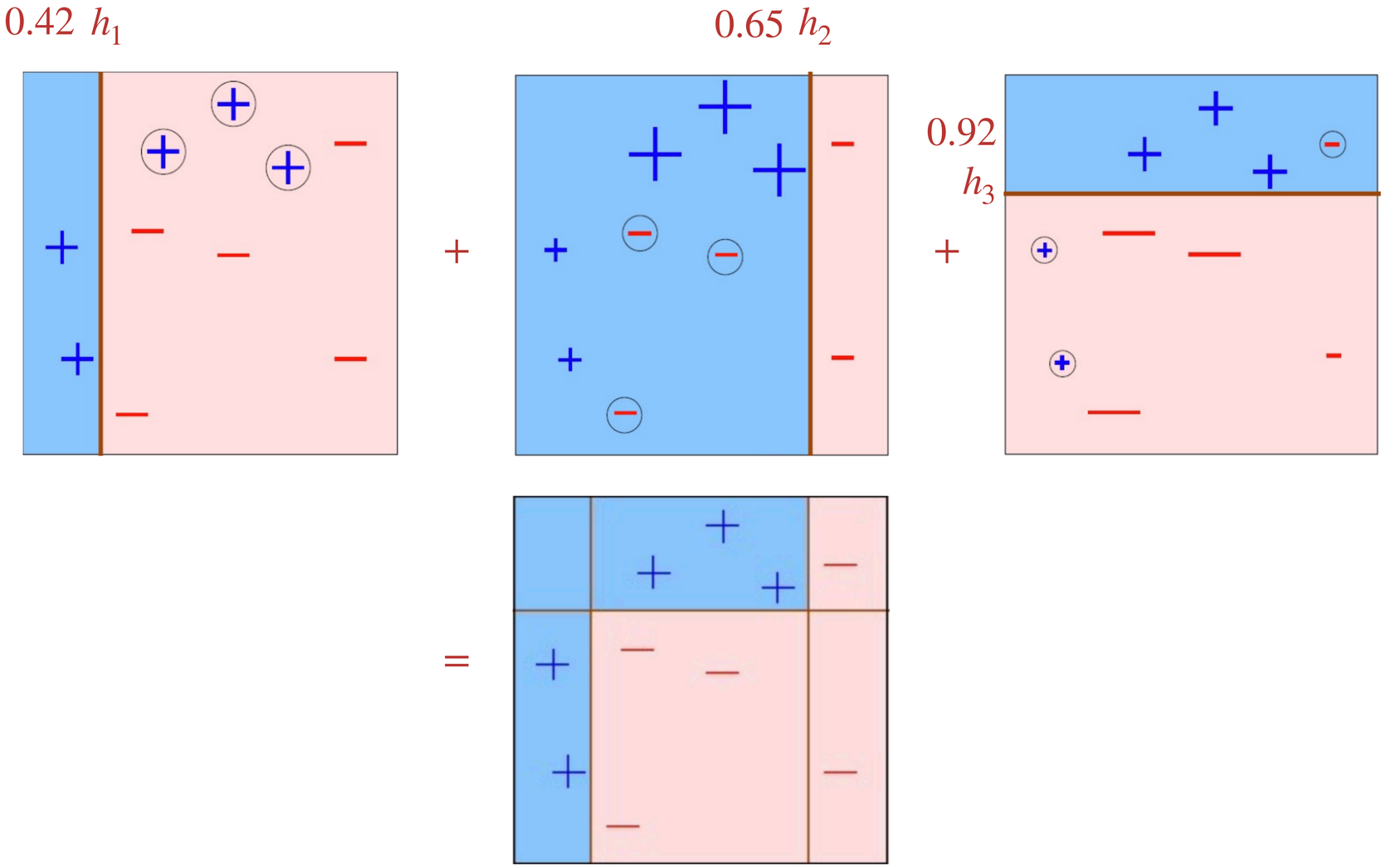




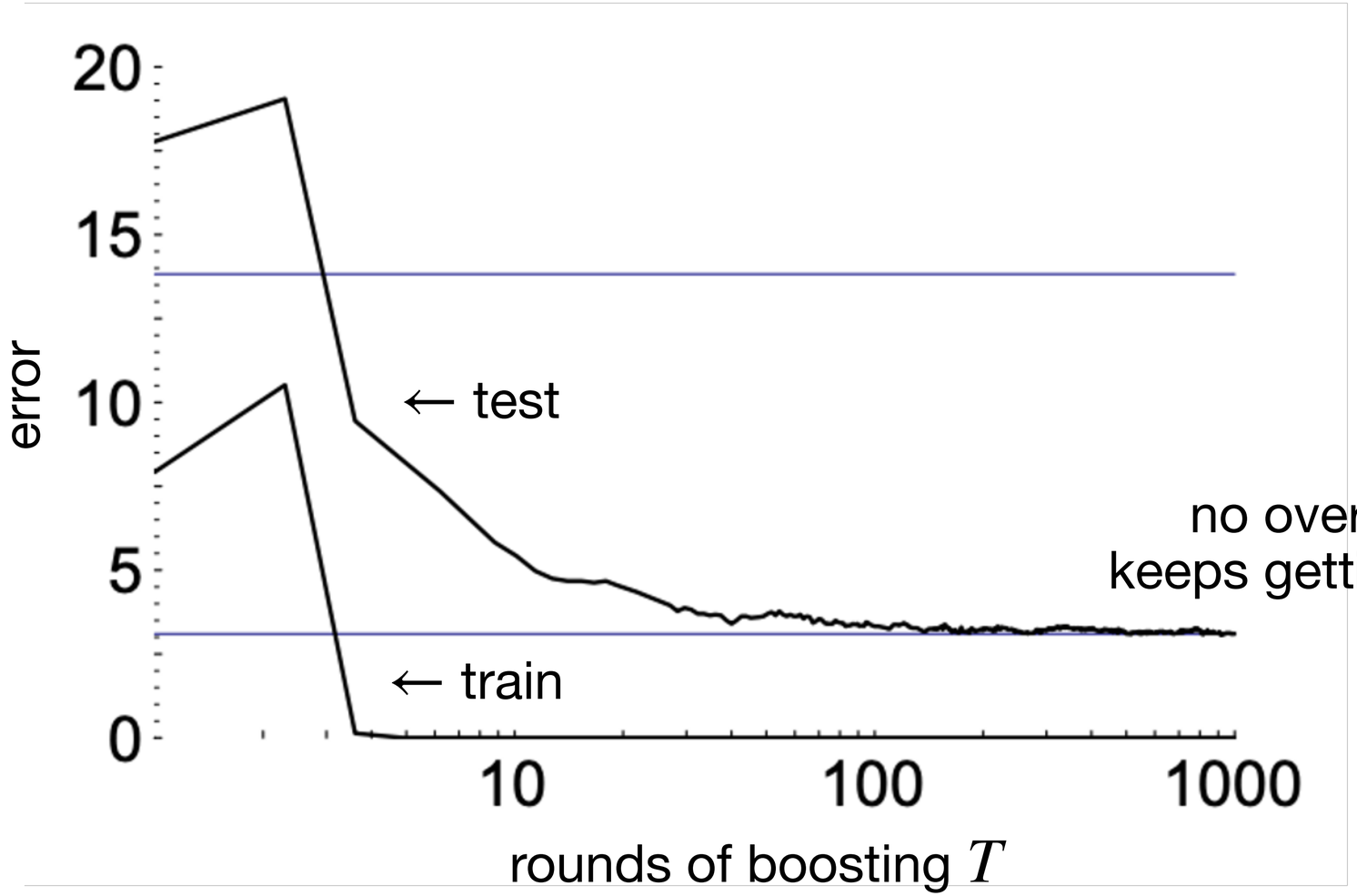
AdaBoost example



AdaBoost example



AdaBoost experiment



no overfitting!
keeps getting better!

Source: http://rob.schapire.net/papers/msri.pdf