Generalization and Capacity Control

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Introduction

Generalization

– Optimize system on a training set and
  expect it to work in future situation.
– Why does it work? When?
– Can we do it better?

Summary

– Generalization: why and when?
– Structural risk minimization.
– Learning algorithms in little pieces.

Generalization is not obvious

Continue the sequence

– 1, 3, 5, 7, ?

Learning by heart versus learning the concept

Generalization is not obvious

Continue the sequence

– 1, 3, 5, 7, ?

Learning by heart versus learning the concept

– But which concept it the right one?

A couple answers

– Odd numbers: 1, 3, 5, 7, 9, 11, 13, 15, 17, . . .

– Prime numbers: 1, 3, 5, 7, 11, 13, 17, 19, 23, . . .

– Numbers palindromic in base two: 1, 3, 5, 6, 9, 15, 17 . . .

– Integers such that $10^n + 19$ is prime: 1, 3, 5, 7, 10, 11, 17, 59, . . .

– Sloane's encyclopedia of numerical sequences
lists 598 well known sequences that start like that.

I. Why can we generalize?

The transductive paradigm

For simplicity, we consider only *a binary classification problem.*

– Given a dataset of $2l$ examples (pattern + class).
– Split examples in two sets L and T of size l.
– Training on the learning set L returns a classifier f.
– Measure learning error μ_L.
– Measure testing error μ_T.

There are $N_{\text{splits}} = C_{2l}^{l} = \frac{2l!}{l!\,l!}$ possible splits.

How many splits yield $\mu_T > \mu_L + \epsilon$?

Let's count them!

Transduction and truth

Ground truth assumption

– "All examples are drawn *independently* from
a single *unknown probability distribution*."
– We cannot test whether this assumption is correct.

Transductive paradigm

– We do not make the ground truth assumption!
– In fact we do not assume anything about the examples!
– But we assume that all splits are equally likely.
– And we consider that success on the testing set is sufficient evidence.

Remark

– The transduction paradigm avoids a lot of technical difficulties.
– Because it describes something more essential. . .

Error vectors

Classification function f.

Examples $(x_1, c_1) \ldots (x_i, c_i) \ldots (x_{2l}, c_{2l})$.

Error vector $m(f) = (0, 0, 0, 1, 0, 0, 1, 0 \ldots, 0, 0, 0)$.

$$\begin{cases} 0 \text{ if } x_i \text{ correctly classified by } f \\ 1 \text{ otherwise} \end{cases}$$

Summarizes everything we need to know about f.
Enough to compute learning error μ_L and testing error μ_T.

When there is a single error vector

Assumption

– Stupid algorithm always returns the same classification function f regardless of the training set L.
– Therefore we always get the same error vector $m = m(f)$

Let's count the splits

– Assume vector contains p ones: $p = 2l\mu(m) = l(\mu_T(m) + \mu_L(m))$.
– There are $C_p^k \, C_{2l-p}^{l-k}$ splits with k ones in the training set.

$$\mathrm{Fr}\left\{\mu_T(m) - \mu_L(m) > \epsilon\right\} = \mathrm{Fr}\left\{\frac{p-k}{l} - \frac{k}{l} > \epsilon\right\}$$

$$= \frac{1}{N_{\text{splits}}} \sum_{p-2k>l\epsilon} C_p^k C_{2l-p}^{l-k}$$

– This is called the *hypergeometric tail*.

Bounds and approximations

We can use a computer and tabulate everything

– Let's define $\epsilon(\mu, l, \eta)$ such that

$$\mathrm{Fr}\left\{\mu_T(m) - \mu_L(m) > \epsilon(\mu(m), l, \eta)\right\} = \eta$$

But some bounds and approximations can be useful

– From (Vapnik, 1982) using Chernoff bounding :

$$\epsilon(\mu, l, \eta) \leq \sqrt{\frac{\log(2/\eta)}{l-1}} \qquad \epsilon(\mu, l, \eta) \leq \sqrt{4\mu\,\frac{\log(2/\eta)}{l}}$$

– Reasonable approximation for l large enough :

$$\epsilon(\mu, l, \eta) \approx \sqrt{4\mu(1-\mu)\,\frac{\log(2/\eta)}{l}}$$

– They all go to zero when l increases.

Decomposition for the general case

$$\mathrm{Fr}\left\{\mu_T - \mu_L > \epsilon\right\} =$$

$$\sum_{L,S} \frac{1}{N_{\text{splits}}} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \times \begin{pmatrix} \mathbb{1}\left\{\mu_T(m_1) - \mu_L(m_1) > \epsilon\right\} \\ \mathbb{1}\left\{\mu_T(m_2) - \mu_L(m_2) > \epsilon\right\} \\ \vdots \\ 0 \\ 1 \\ \vdots \\ \mathbb{1}\left\{\mu_T(m_{\mathcal{N}}) - \mu_L(m_{\mathcal{N}}) > \epsilon\right\} \end{pmatrix}$$

- The sum runs over all the possible splits.
- The green vector indicates which error vector is produced by the classifier returned by running learning algorithm on that split.
- The purple vector indicates which error vectors have an error deviation greater than ϵ.

Gross bound for the general case

Bound the green vector with a vector with all ones!
This sometimes called the *union bound*.

$$\mathbf{Fr}\left\{\mu_T - \mu_L > \epsilon(\mu, l, \eta)\right\} \leq \eta\,\mathcal{N}(\mathcal{F}, \mathcal{D})$$

Equivalently

$$\mathbf{Fr}\left\{\mu_T - \mu_L > \epsilon\left(\mu, l, \frac{\eta}{\mathcal{N}(\mathcal{F}, \mathcal{D})}\right)\right\} \leq \eta$$

$\mathcal{N}(\mathcal{F}, \mathcal{D})$ is the important quantity.
– Family $\mathcal{F}$ contains all classifiers possibly returned by the algorithm.
– $\mathcal{N}(\mathcal{F}, \mathcal{D})$ counts the distinct error vectors produced by $f \in \mathcal{F}$.

With probability $1 - \eta$

$$\mu_T - \mu_L \leq \epsilon\left(\mu, l, \frac{\eta}{\mathcal{N}(\mathcal{F}, \mathcal{D})}\right) \approx \sqrt{4\mu(1-\mu)\,\frac{\log(2/\eta) + \log \mathcal{N}(\mathcal{F}, \mathcal{D})}{l}}$$

The failure mode

– Obviously $\mathcal{N}(\mathcal{F}, \mathcal{D}) \leq 2^{2l}$.

What is happening when $\mathcal{N}(\mathcal{F}, \mathcal{D}) = 2^{2l}$?

– All the possible error vectors are represented.
– Split the classifiers from $\mathcal{F}$ into groups of classifiers that perform identically on the learning set.
– Each group contains classifiers that produce all possible error patterns on the testing set.
– Classifiers from a same group perform identically on the learning set. Short of additional information, the trainign algorithm cannot know which ones work well on the testing set.
– No generalization guarantees.
– But we can be lucky. . . sometimes. . .

The finite case

Assumption

"The family of classifiers $\mathcal{F}$ is finite."

Consequences

– $\mathcal{N}(\mathcal{F}, \mathcal{D}) \leq \text{Card}(\mathcal{F}) < 2^{2l}$ when l is large enough.

– $\mu_T - \mu_L \lesssim \sqrt{4\mu(1-\mu)\,\frac{\log(2/\eta)}{l} + \frac{\log(\text{Card}\mathcal{F})}{l}}$.

– We can generalize.

– We need $l \gg \log \text{Card}(\mathcal{F})$.

The infinite case

Vapnik-Chervonenkis combinatorial lemma

Let $m_{\mathcal{F}}(l) = \max_{\{x_1, c_1 \ldots x_l, c_l\}} \mathcal{N}(\mathcal{F}, \{x_1, c_1 \ldots x_l, c_l\})$.

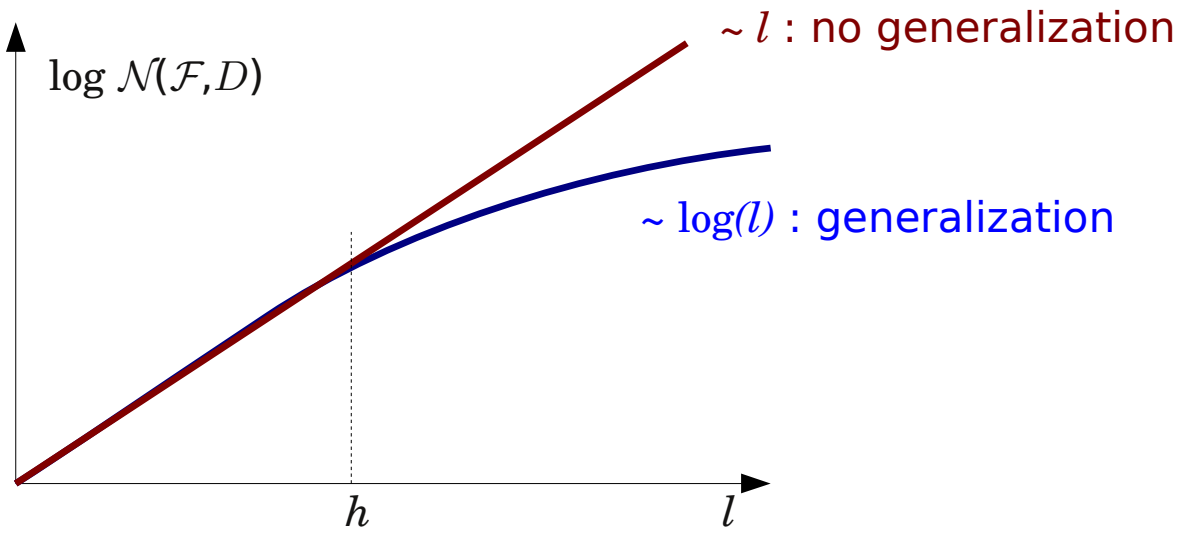
- Either $m_{\mathcal{F}}(l) = 2^l$ for all l.
- Or $m_{\mathcal{F}}(l) \leq \left(\frac{le}{h}\right)^h$ where h is the last value such that $m_{\mathcal{F}}(h) = 2^h$.

– Quantity h is called the Vapnik-Chervonenkis of the family $\mathcal{F}$.
It measures the "capacity" of a family of functions.

(Vapnik and Chervonenkis, 1968) (Sauer, 1972)
Some people unfairly call this lemma "Sauer's lemma".

The infinite case

What is true for $m_{\mathcal{F}}(l)$ is true for $\mathcal{N}(\mathcal{F}, \mathcal{D})$.



– We cannot generalize when $h = \infty$.

– Otherwise $\mu_T \lesssim \mu_L + \sqrt{4\mu(1-\mu)\left[\frac{\log(2/\eta)}{l} + \frac{h}{l}\log\frac{2le}{h}\right]}$

– We can generalize when $h < \infty$.

– We need $l \gg h$.

VC dimension versus other capacity measures

Results with VC dimension

- Impressive achievements despite gross bounding technique:
  - Infinite VC dimension $\Longrightarrow$ no generalization guarantees.
  - Finite VC dimension $\Longrightarrow$ generalization when l is large enough.
- Price of the gross bounding technique:
  - Simple bounds on $\mu_T - \mu_L$ are way too large.

Annealed VC entropy $\log \mathcal{N}(\mathcal{F}, \mathcal{D})$

- This is a quantity that matters more.
- Better estimates of this quantity improves $\mu_T - \mu_L$ bounds.
- Lots of sophisticated theoretical works.
  - data dependent bounds, localized bounds, ...

Union bound

- Maybe the coarsest bound here.
- Little progress improving on that.

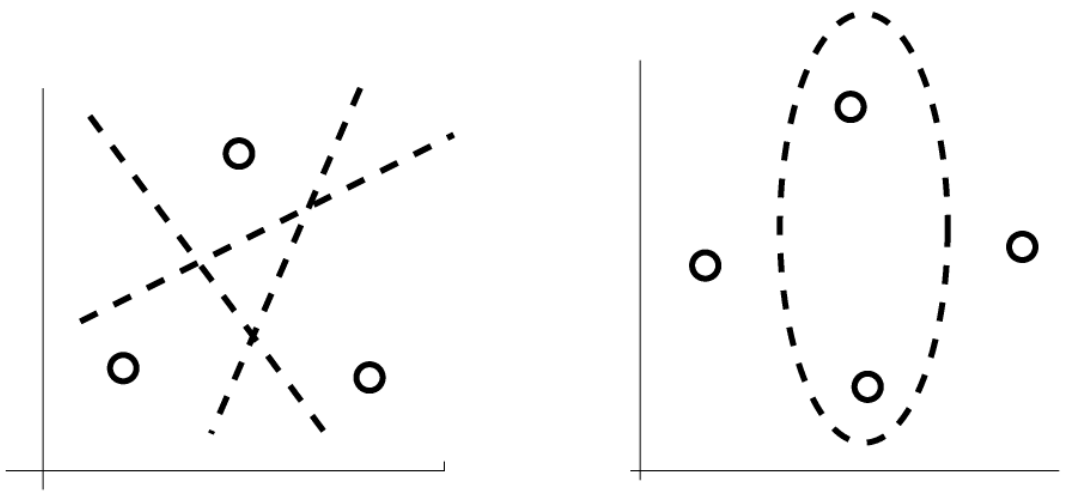
Capacity = number of parameters

The VC dimension of the set of linear discriminant functions

$$f_{w,b}(x) = \mathbb{1}\left\{w^\top x + b \geq 0\right\} \quad x, w \in \mathbb{R}^d \quad b \in \mathbb{R}$$

is equal to the number of parameters

$$h = d + 1\,.$$

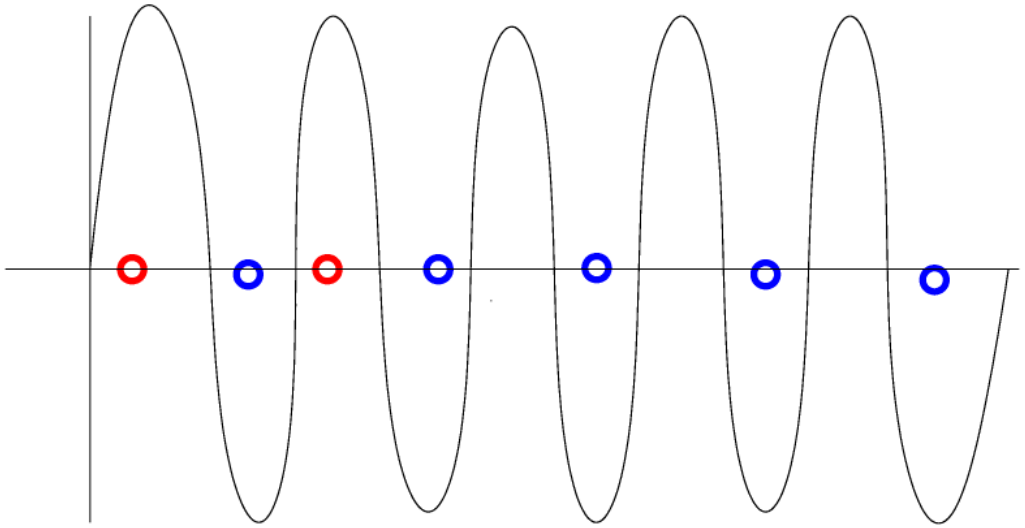


Capacity $\gg$ number of parameters

The VC dimension of the set of functions

$$f_w(x) = \mathbb{1}\{sin(wx) \geq 0\} \quad x, w \in \mathbb{R}$$

is infinite



Capacity $\ll$ number of parameters

Assume the patterns $x_1 \ldots x_{2l}$ are known beforehand.
The classes are unknown.
Let $R = \max \|x_i\|$.

We say that a hyperplane

$$w^\top x + b \quad w, x \in \mathbb{R}^d \quad \|w\| = 1$$

separates patterns with margin Δ if

$$\forall i = 1 \ldots 2l \quad |w^\top x_i + b| \geq \Delta$$

The family of Δ-margin separating hyperplanes has

$$\log \mathcal{N}(\mathcal{F}, \mathcal{D}) \leq h \log \frac{2le}{h} \quad \text{with} \quad h \leq \min \left\{ \frac{R^2}{\Delta^2}, d \right\} + 1$$

Razors

Occam's razor

– When reasoning, "*entities must not be multiplied beyond necessity*".
– Means that the simplest solution is often the correct one.

Capacity and Occam's razor

– What matters is not the complexity of the final classifier,
but the capacity of the family of classifiers we consider.
– Capacity is not the same as the number of parameters.

Vapnik's razor

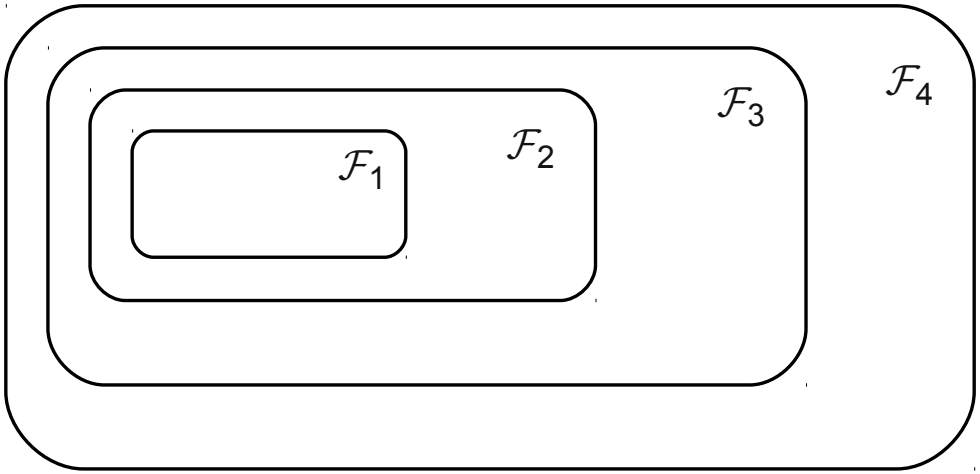
– "*When solving a problem, avoid solving*
a more complicated problem as an intermediate step."
– The more complicated problem needs a higher capacity $\mathcal{F}$.
– Therefore one would need more examples.

II. Structural Risk Minimization, etc.

Structural Risk Minimization

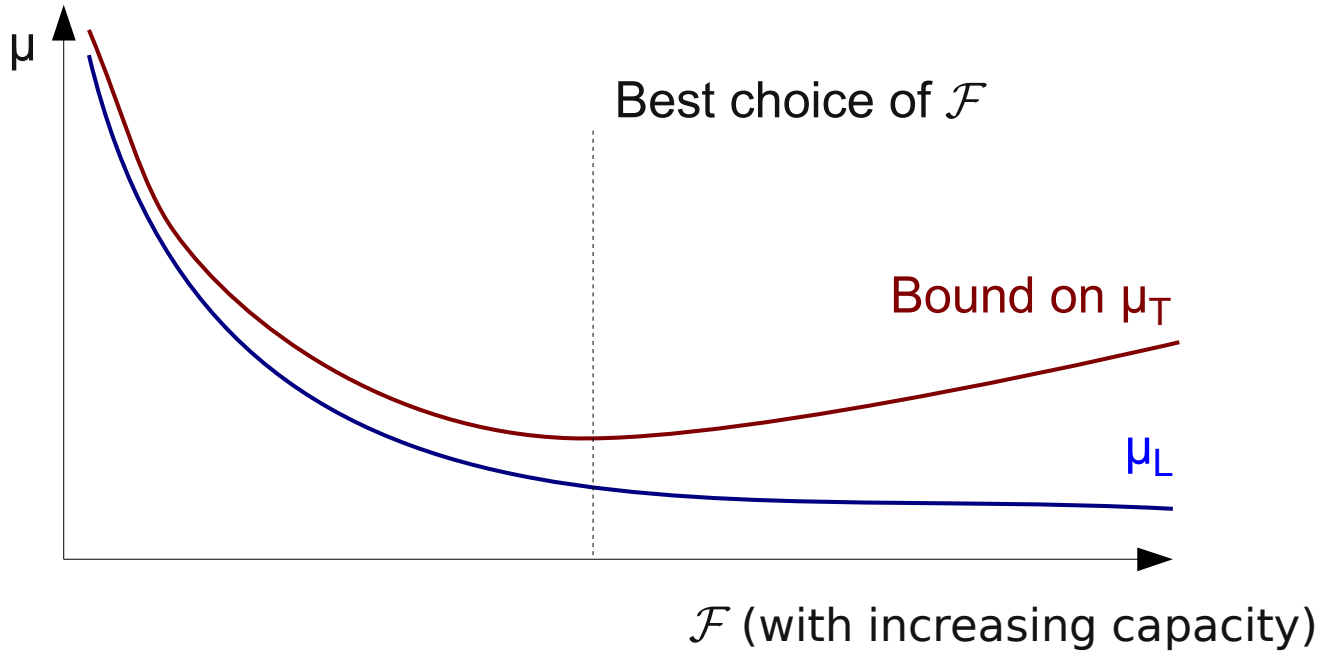
Consider an embedded sequence of families of functions

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \ldots$$



This is called a structure.

Structural Risk Minimization



There is a best family in the sequence for each l.

Model Selection

1. Define a capacity control structure.

2. Optimize for each structure member.

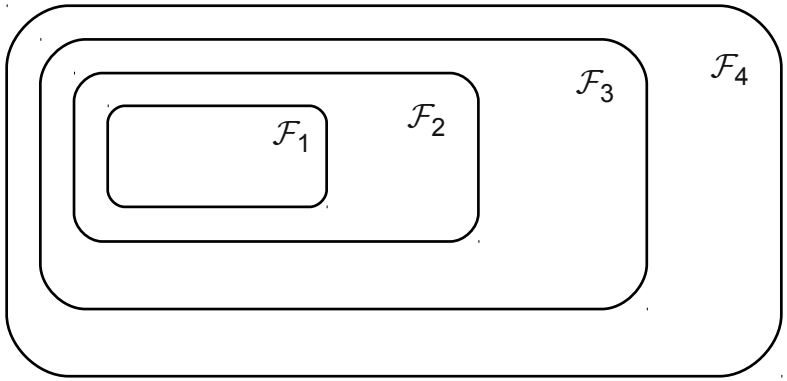
3. **Choose one.**
   - *Empirically*:

Holdout	(looses examples)
Leave-one-out	(high variance)
K-Fold CV	(few results)

   - *Theoretically*:

Standard VC bounds	($\boldsymbol{p < 1000}$)
Advanced VC bounds	($\boldsymbol{p < 1}$)
Effective VC bounds	(compute intensive)
Automatic	(dream)

What is a "structure"

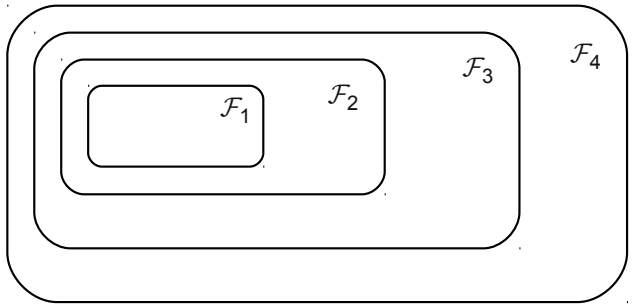


The structure defines a preorder on the functions.

All other things being equal:
– We'll prefer a function from $\mathcal{F}_1$ over a function of $\mathcal{F}_2$.
– We'll prefer a function from $\mathcal{F}_2$ over a function of $\mathcal{F}_3$.
– We'll prefer a function from $\mathcal{F}_3$ over a function of $\mathcal{F}_4$.
– etc.

Very similar to a Bayesian prior!

Regularizers



Let $C_1 < C_2 < C_3 < C_4 < \ldots$
Define $\mathcal{F}_i = \{f \ : \ \Omega(f) \leq C_i\}$.

The function $\Omega(f)$ expresses preferences.
We prefer f_1 over f_2 when $\Omega(f_1) < \Omega(f_2)$.

Resulting learning algorithm:

$$\min_f \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)) \ + \ \lambda \Omega(f)$$

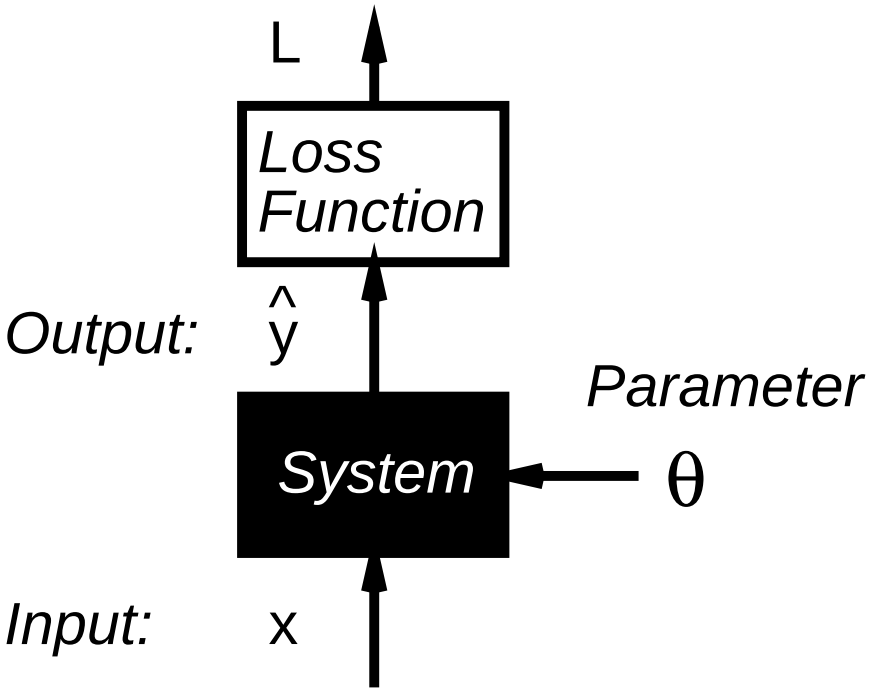
– Regularizer $\Omega(f)$ expresses preferences.
– Hyperparameter λ define their strength.
– Choosing λ amounts to choosing a $\mathcal{F}_i$.
– Must adjust λ for each l, for instance using cross-validation.

III. Learning algorithms in little pieces

A. Representation

Representation	**Parametric vs. Kernels** **Linear vs. Non-Linear**
Capacity Control	Explicit via architecture Explicit via feature selection Explicit via regularizers Implicit via optimization Implicit via margins
Operational Considerations	Loss functions Online vs. offline Budget constraints
Computational Considerations	Exact algos for *small data.* *Stochastic algos for* big data. Parallel algos.

Representation - Parametric



Parametric:

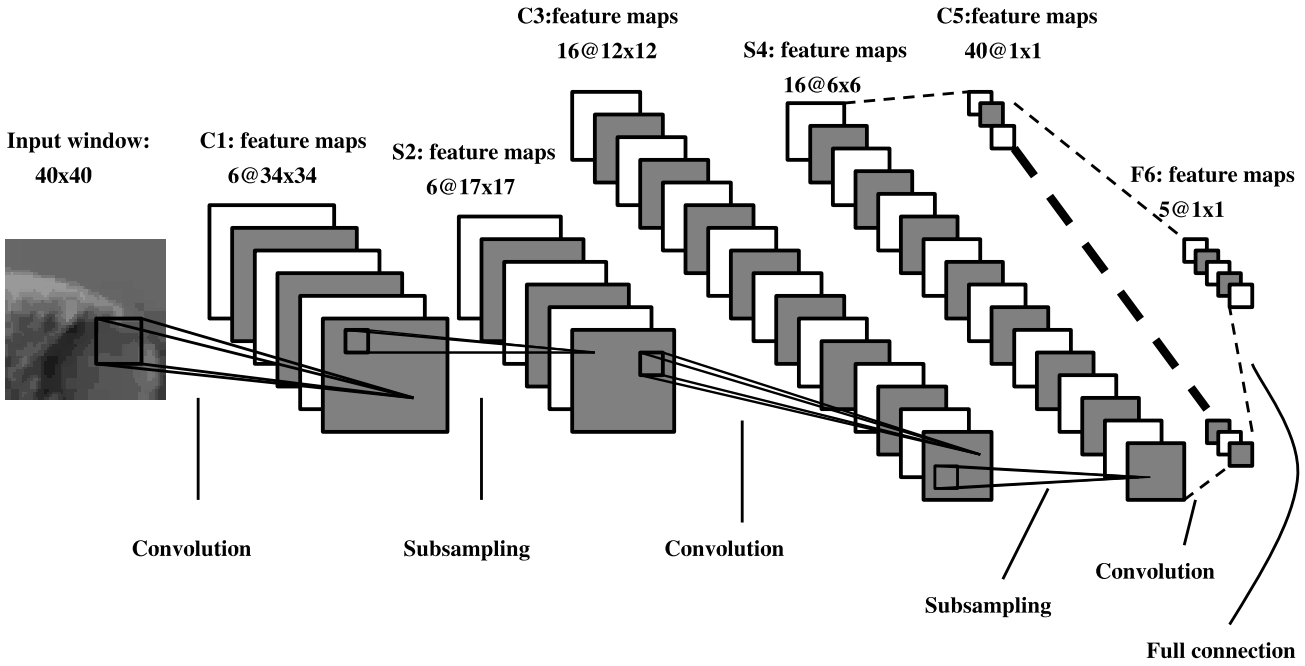
θ is a vector.

Non Parametric:

θ belongs to a bigger space.

Representation - Networks

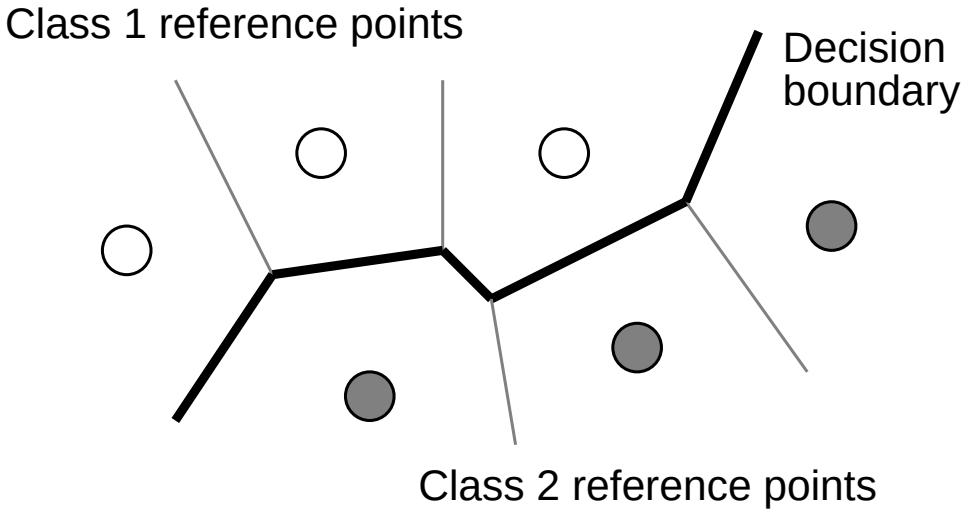
Example: Convolutional Network



- Very good for *image and signal*.
- Learning algorithms are *delicate* (non-linear, non-convex.)

Representation - Centroids

Examples: KMeans, LVQ



- Fast algorithms for relatively low input dimension.
- Generally more difficult for high input dimension.

Representation - Mixtures

Example: Mixture of Gaussians

- Fast algorithms for relatively low input dimension.
- Generally more difficult for high input dimension.

Example: Mixture of Experts, Voting Schemes.

- Divide and conquer.
- Capacity control more difficult.

Representation - Kernels

Suitable for θ in function space.

- Decision function uses the training examples x_i.

$$\hat{y}(x) = \sum_i \alpha_i K(x_i, x) + b$$

- Kernel function is a dot-product in some large space.

$$K(x, y) = \langle \Phi(x), \Phi(y) \rangle$$

- Algorithms must only use $K(x, y)$, not $\Phi(x)$.
- Sparsity is desirable.
- See next lecture!

B. Loss Functions

Representation	Parametric vs. Kernels Linear vs. Non-Linear
Capacity Control	Explicit via architecture Explicit via feature selection Explicit via regularizers Implicit via optimization Implicit via margins
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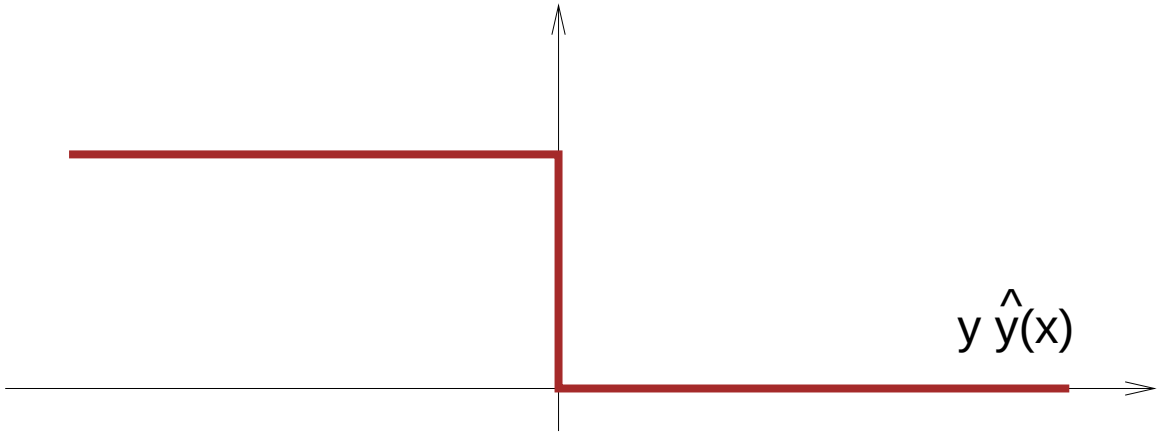
Pattern Recognition Losses - Ideal

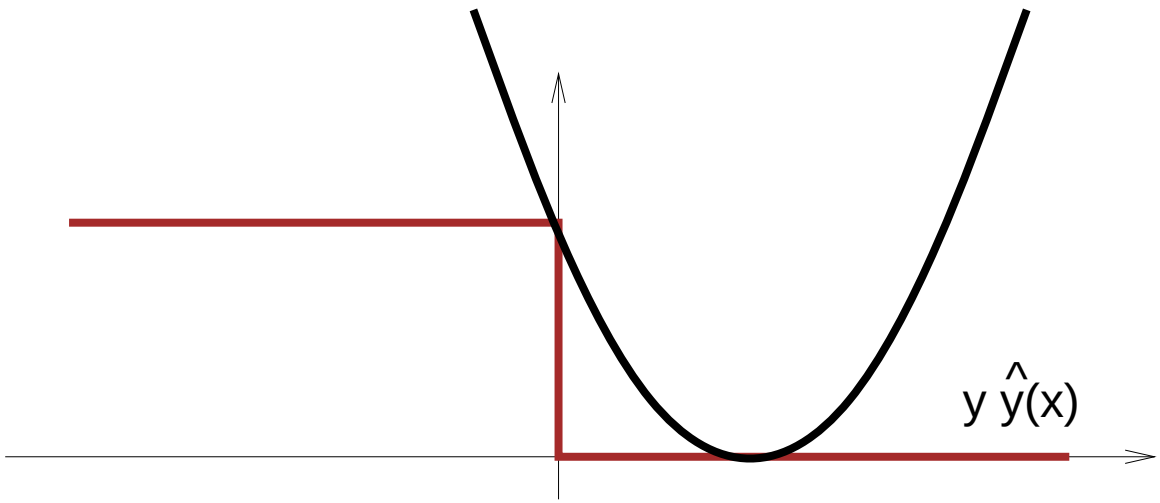
- Example x has class $y = \pm 1$.
- Mistake if y and $\hat{y}(x)$ have different signs.
- Minimize number of mistakes?



Pattern Recognition Losses - Quadratic

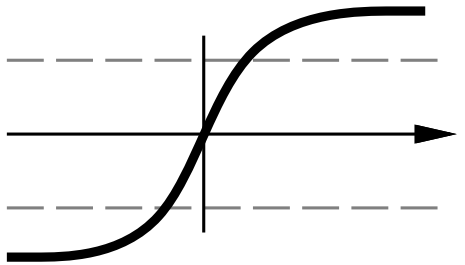
$$L = (y - \hat{y}(x))^2$$

- Approximate posterior probabilities $P(y|x)$.
- Convex, easy to optimize.
- Bound problems.

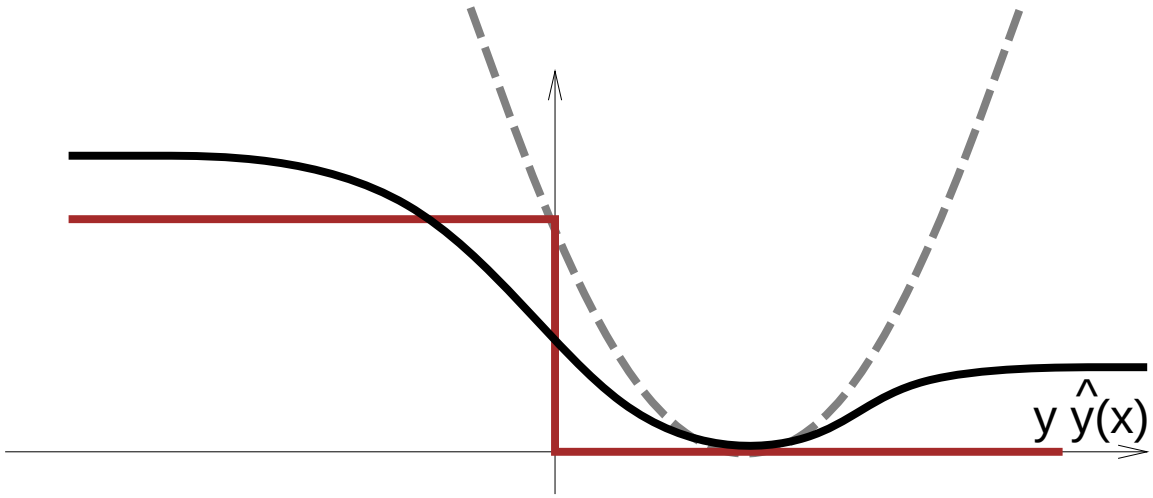


Pattern Recognition Losses - Sigmoïd

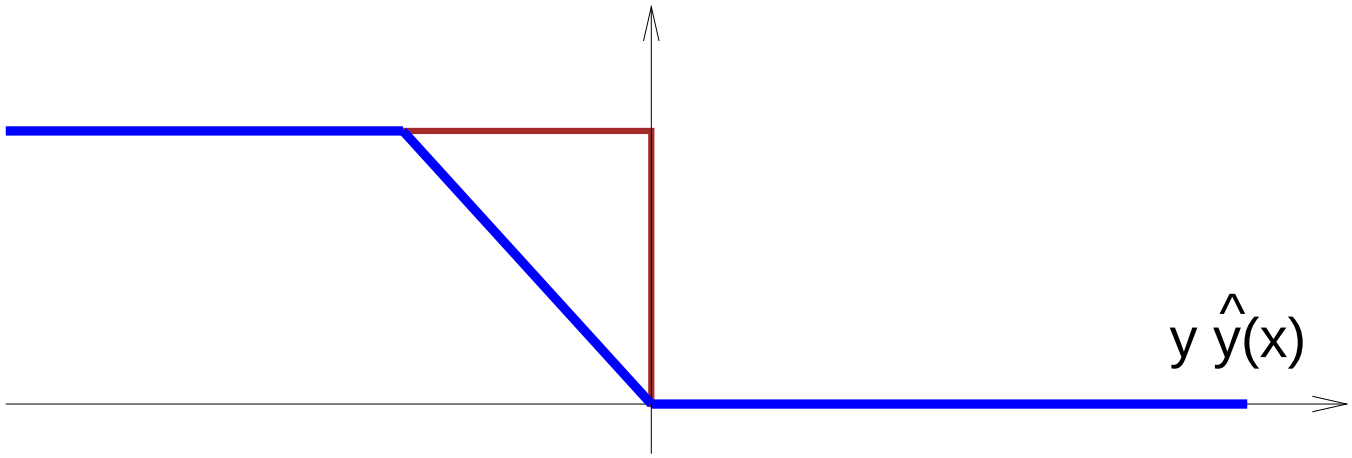
$$L = (\ y - 1.7 \tanh(\hat{y}(x))\ )^2$$



- Solves bound problems.
- Non-convex, more difficult to optimize.
- Still Approximate posterior probabilities $P(y|x)$.



Pattern Recognition Losses - LVQ...



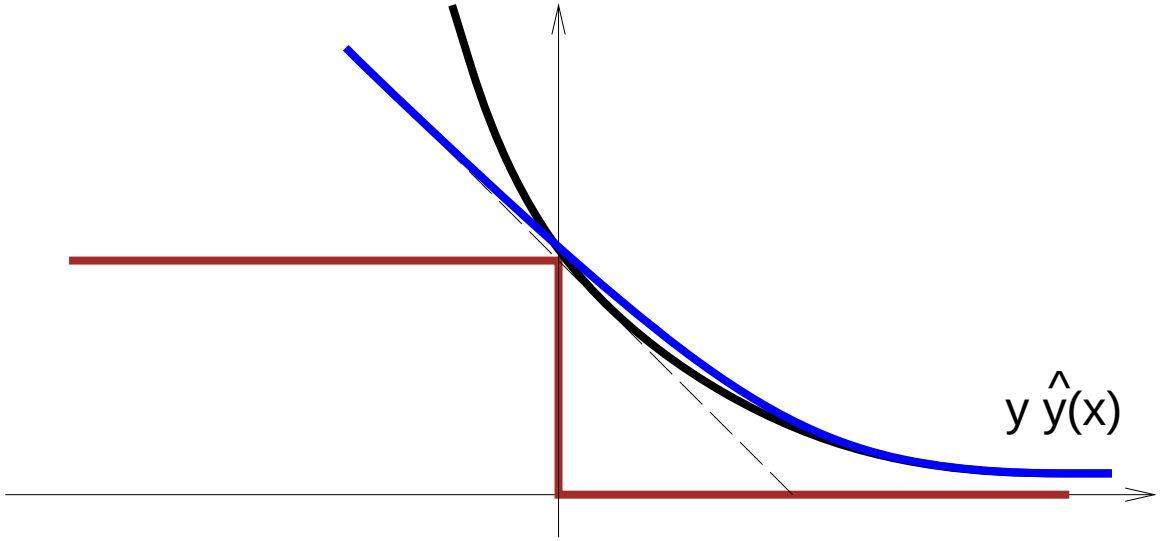
Centroid Representation + LVQ loss $\longrightarrow$ LVQ algorithm.

$$\hat{y}(x) = \frac{(x - w^+)^2 - (x - w^-)^2}{\delta(x - w^-)^2}$$

w^- : closest centroid.
w^+ : closest centroid w/correct class.

Pattern Recognition Losses - Exp/Log

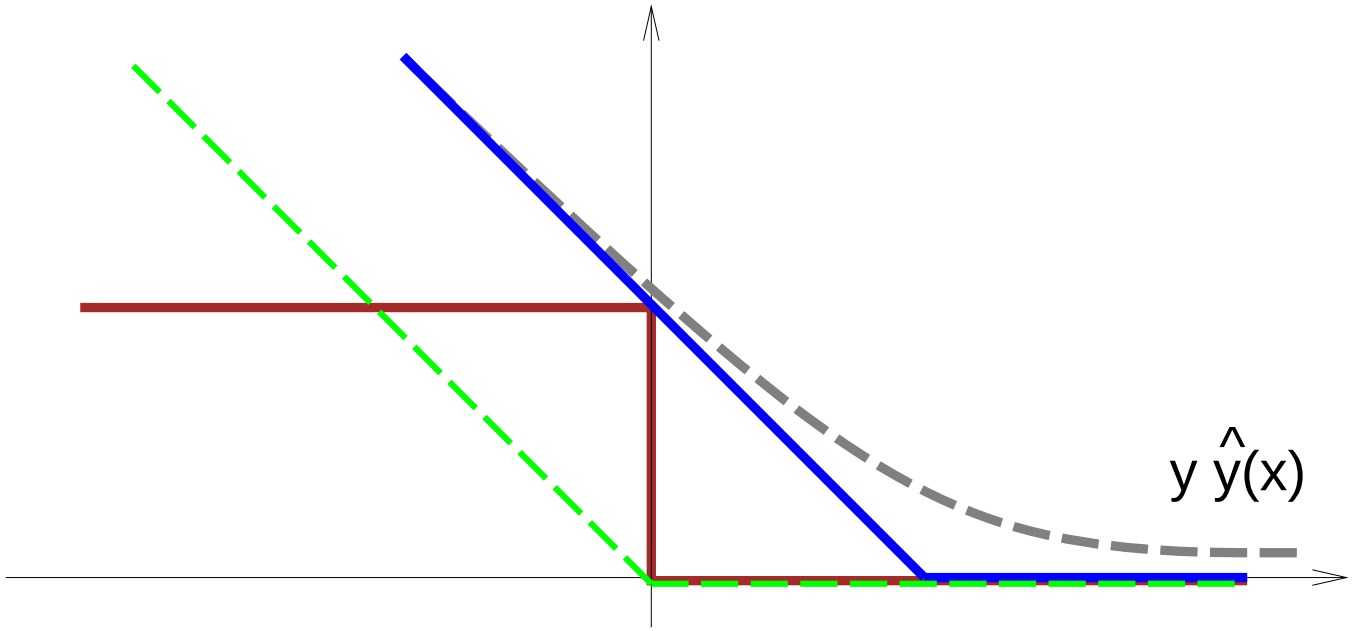
- Approximate posterior probabilities $P(y|x)$.
- Convex.



- **ExpLoss** $\longleftrightarrow$ Boosting,. . .
- **LogLoss** $\longleftrightarrow$ Maximum likelihood for $\mathrm{P}\{Y|X\}$.

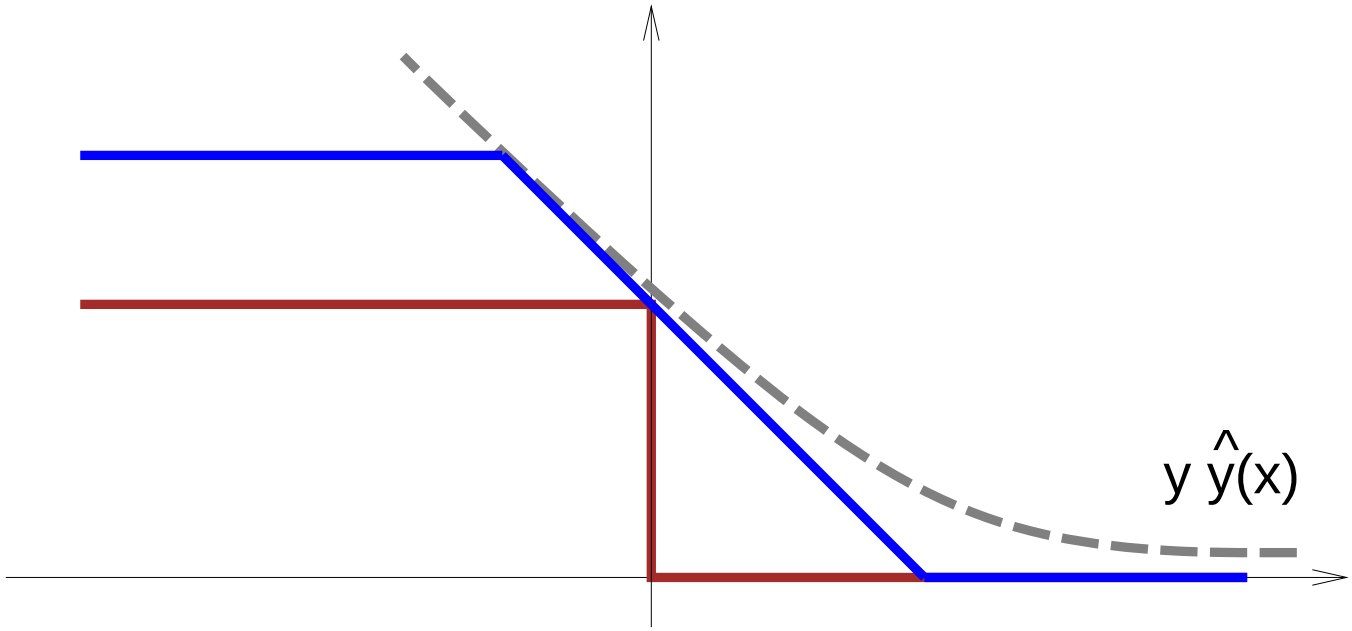
Pattern Recognition Losses - Hinge

- Does not approximate probabilities.
- Convex.

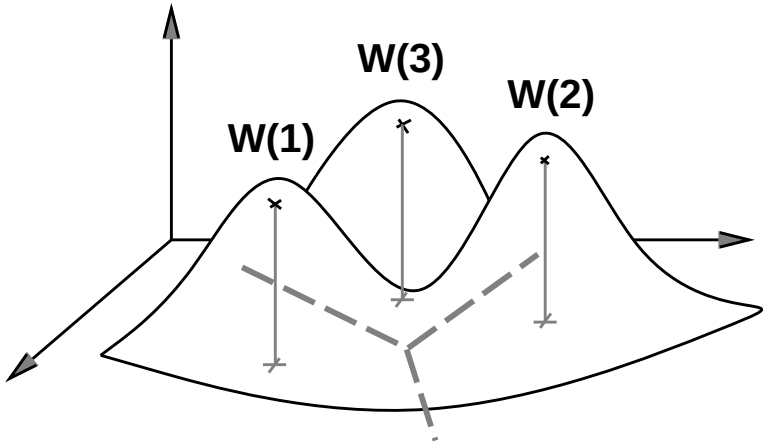


- **PerceptronLoss** $\longleftrightarrow$ Perceptron,. . .
- **HingeLoss** $\longleftrightarrow$ SVM,. . .

Pattern Recognition Losses - Ramps



Clustering Losses - VQ

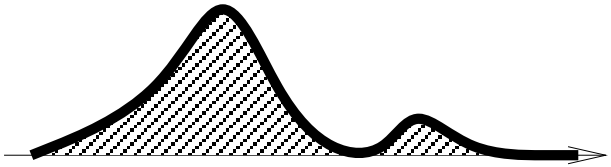


Minimize quantization error:

$$L = \min_k (x - w_k)^2$$

Example: k-Means.

Density Losses - KL, Hellinger



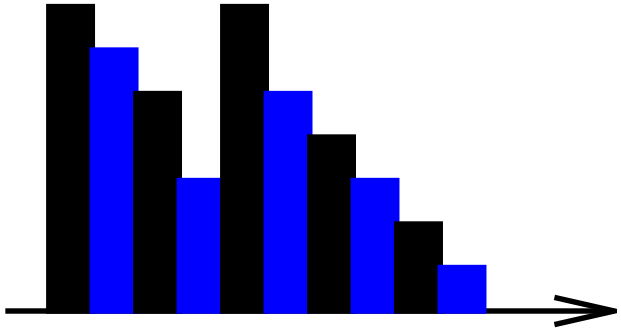
Optimize:

$$L = -\log(\hat{y}(x))$$

Normalization:

$$\int \hat{y}(x)dx = 1 \quad \longrightarrow P(x)$$
$$\sum_k \hat{y_k}(x) = 1 \quad \longrightarrow P(y|x)$$

Most statistical systems.



Compare histograms:

$$L = \sum_k \left(\sqrt{\hat{y_k}(x)} - \sqrt{y_k}\right)^2$$

Novelty detection.

C. Capacity Control Strategies

Representation	Parametric vs. Kernels Linear vs. Non-Linear
Capacity Control	**Explicit via architecture** **Explicit via feature selection** **Explicit via regularizers** **Implicit via optimization** **Implicit via margins**
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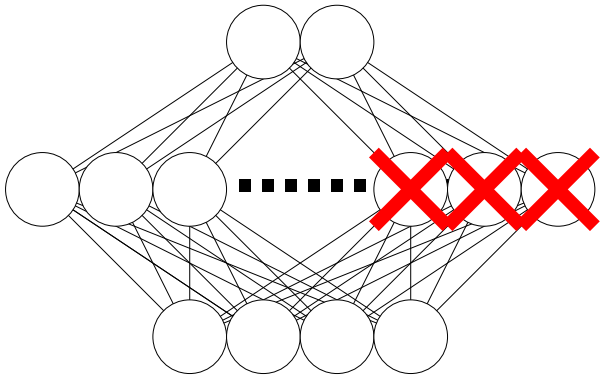
Capacity Control - Explicit

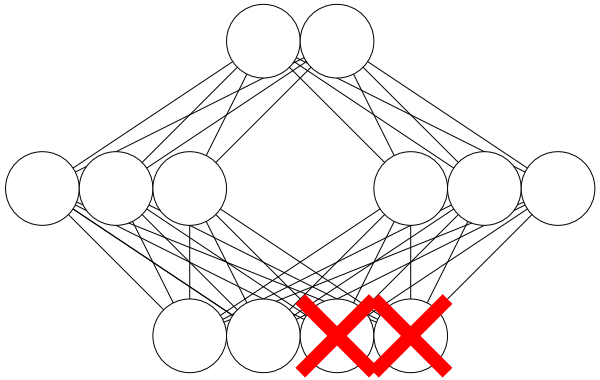


via Architecture

Architecture changes capacity.

Model selection.

Search algorithm.

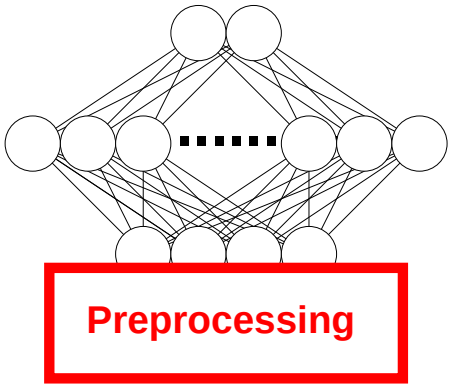


via Feature Selection

Feature selection.

Search algorithms.

Capacity Control - Explicit



via Preprocessing

Handcrafted features.

Dimensionality reduction.

Smoothing.

$$\min \left\{ \begin{array}{c} \mathbb{E}_z L(z,w) \\ +\lambda \Omega(w) \end{array} \right.$$

via Regularization

Hyperparameter λ.

Ω	
$\|w\|^2$	Ridge, ...
$\|w\|$	Lasso, ...
$\|\partial_x \hat{y}(x)\|^2$	Smoothness, ...
$\|T_\alpha w\|^2$	Tangent prop

Capacity Control - Implicit

Example:

- Non-Linear Neural Network.
- 10^5 to 10^6 parameters.
- Poor optimizer (stochastic gradient)

This controls capacity via:

- Initial parameters w_0.
- Learning rate limits $\|w - w_0\|^2$.
- Algorithm inefficencies $\|\partial_x \hat{y}(x)\|^2$.
- Early stopping.

The capacity control levers are mixed
with the delicate optimization settings.

Capacity Control - Bayesian

Bayesian priors also express a preorder on the functions f.
– but also define a numerical strength associated with preferences.

Bayes framework does not suggest a λ hyperparameter.
– But the prior numerical strength can be more or less peaky.
– Often the prior peakiness is controlled by an hyperparameter that itselfs obeys its own prior distribution, etc.

Bayesian averaging has no equivalent here!