FUNDAMENTALS OF LEARNING AND INFORMATION PROCESSING

SESSION 17: STATISTICAL MACHINE LEARNING (VII)

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Regularized Loss Minimization

Regularized Loss Minimization (RLM)

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  RLM and SRM We can define a sequence of hypothesis classes, $\mathscr{H}_1 \subset \mathscr{H}_2 \subset \mathscr{H}_3 \ldots$, where $\mathscr{H}_i = \{\omega : \|\omega\| \leq i\}$. If the sample complexity of each $\mathscr{H}_i$ depends on i, then the RLM is similar to SRM for this sequence of nested classes.

- **Stabilizer**: Tikhonov regularization makes the learner stable w.r.t. small perturbation of the training set, which in turn leads to better generalization.

Stability

Given a training set $S = (z_1, \cdots, z_{i-1}, z_i, z_{i+1}, \cdots, z_m)$ and an additional example z', let $S^{(i)}$ be the training set obtained by replacing $z_i \in S$ by z', namely $S^{(i)} = (z_1, \cdots, z_{i-1}, z', z_{i+1}, \cdots, z_m)$ and let $U(m)$ be the uniform distribution over $[m]$. Let $\epsilon : \mathcal{N} \mapsto \mathcal{R}$ be a monotonically decreasing function. We say that a learning algorithm A is On-Average-Replace-One-Stable with rate $\epsilon(m)$ if every distribution $\mathcal{D}$:

$$\mathop{\mathrm{E}}_{(S,z') \sim \mathcal{D}^{m+1}, i \sim U(m)} [l(A(S^{(i)}, z_i)) - l(A(S), z_i)] \leq \epsilon(m)$$

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- Informally: an algorithm A is stable if a small change of its input S will lead to a small change of its output hypothesis.
- Need to specify what is "small change of input" and what is "small change of output".

□

Stable Rules Do Not Overfit

if A is *on-average-replace-one-stable* with rate $\epsilon(m)$ then

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- The proof follows from the definition of *stability*.

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Tikhonov Regularization as Stabilizer

Assume that the loss function is convex and ρ-Lipschitz. Then, the RLM rule with the regularizer $\lambda\|\omega\|^2$ is on-average-replace-one-stable with rate $\frac{2\rho^2}{\lambda m}$. It follows that:

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Similarly, for convex, β-smooth, and non-negative, the loss rate is $\frac{48\beta C}{\lambda m}$, with C is the upper bound on $\max_z l(\vec{0}, z)$, where $\omega = \vec{0}$.

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Notes.

- The proof relies on the notion of strong convexity and is omitted here.

□

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The expected risk of a learning algorithm A can be rewritten as

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- λ controls the trade-off between above two terms.

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  $L_S(A(S)) \leq L_S(A(S)) + \lambda\|A(S)\|^2 \leq L_S(\omega^*) + \lambda\|\omega^*\|^2$.
- Taking expectation of both sides with respect to S and noting that $E_S[L_S(\omega^*)] = L_{\mathscr{D}}(\omega^*)$, we obtain that $E[L_S(A(S))] \leq L_{\mathscr{D}}(\omega^*) + \lambda\|\omega^*\|^2$.
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- The stability term decreases as λ increases, and the empirical risk increases with λ. So a trade-off is needed.

□

The Regularization Path

The RLM rule as a function of λ is $\omega(\lambda) = \text{argmin}_\omega L_S(\omega) + \lambda\|\omega\|^2$. It can be seen as a *Pareto* objective: minimize both $L_S(\omega)$ and $\|\omega\|^2$.

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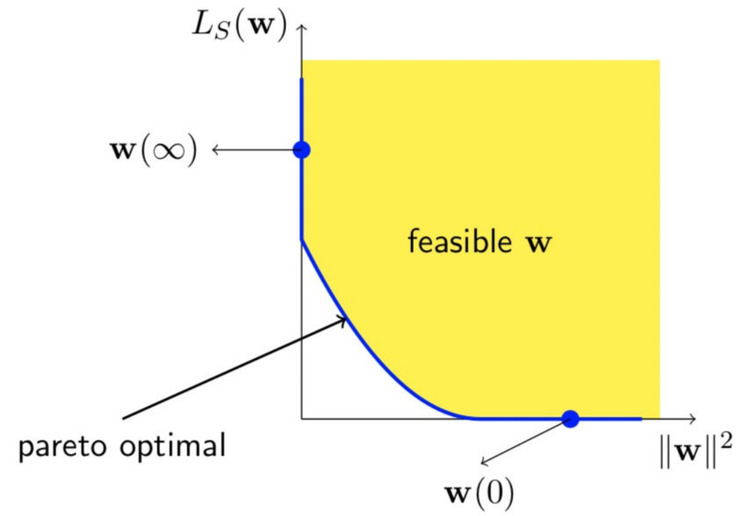
Validation calculate several *Pareto* optimal points on the regularization path (by varying λ) and use validation set to choose the best one.

□



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The expected risk of a learning algorithm A can be rewritten as

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- Here, we learn d parameters but the *sample complexity* depends on the norm of $\|\omega\|$ and on the Lipschitzness/smoothness, rather than on d.
- Which approach is better depends on the properties of the distribution.

□

Support Vector Machine

Binary Classification

Consider a binary classification problem:

Hypothesis $\mathscr{H}$ the function set as:

$$h(x) = \begin{cases} 1 & \text{when } f(x) > 0 \\ -1 & \text{when } f(x) < 0 \end{cases}$$

Loss Function The number of times h get incorrect results on the sample.

$$L(h(x), y) = \sum_{i=1}^{n} l^{0-1}(h(x_i) \neq y_i) \approxeq \sum_{i=1}^{n} l(f(x_i), y_i)$$

Training by Optimization Gradient descent is possible if both $h(x)$ and $f(x)$ are differentiable, otherwise difficult.

Loss Function

How to choose a differentiable function to approximate l^{0-1}?

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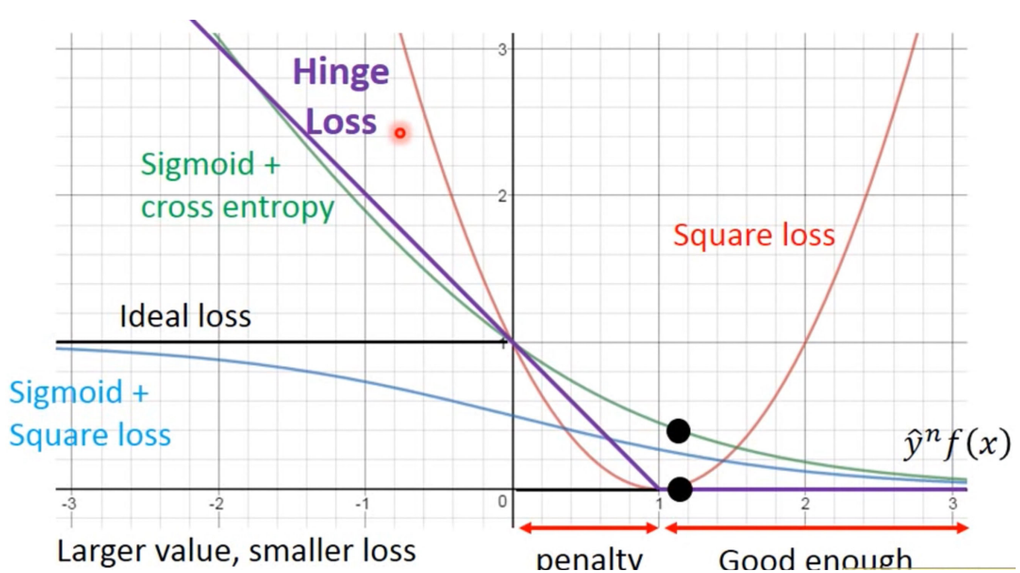

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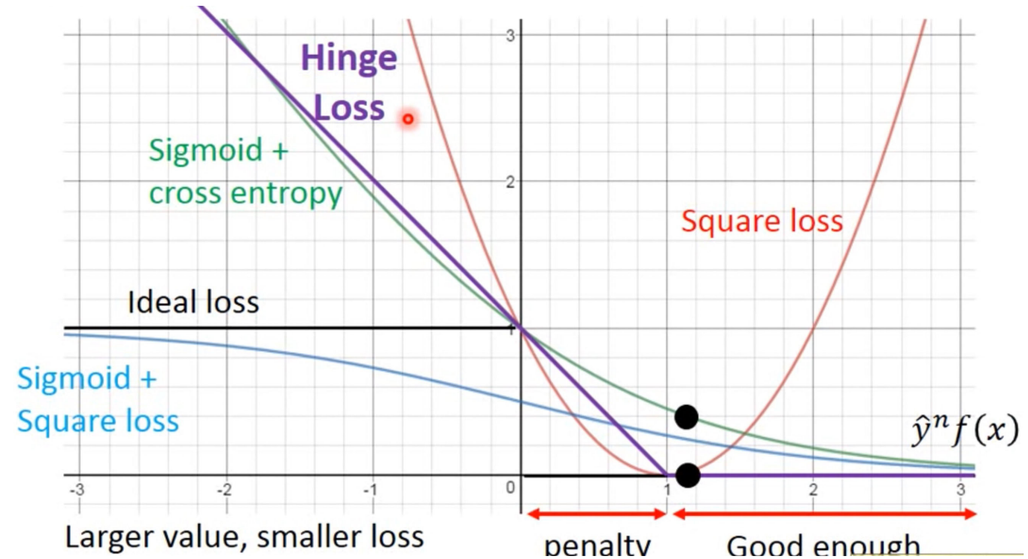

Squared Loss.

$$l(f(x_i), y_i) = (y_i f(x_i) - 1)^2$$

- Intuitively, it wants to achieve:

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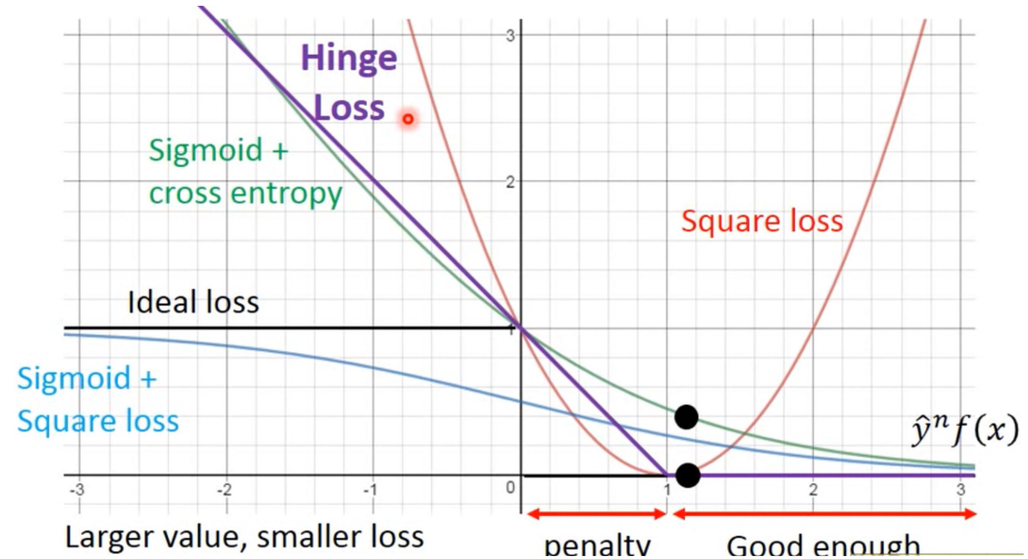

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- It penalizes the very correct examples where $y_i f(x_i) \gg 1$

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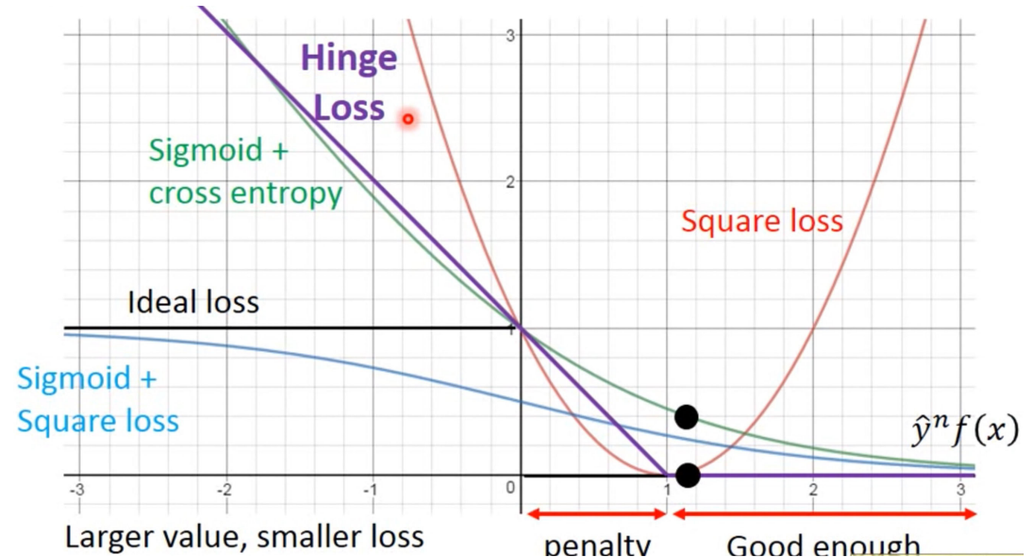

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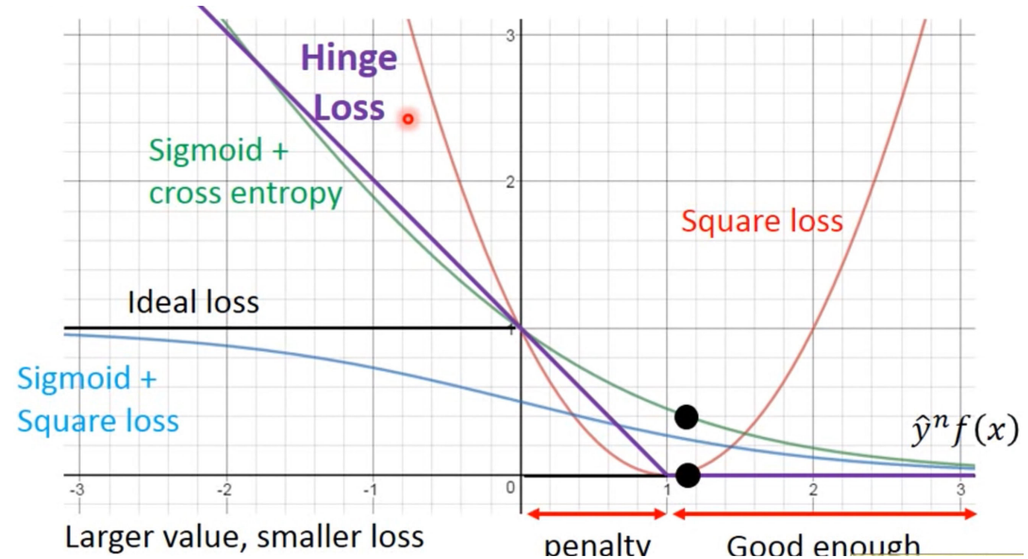

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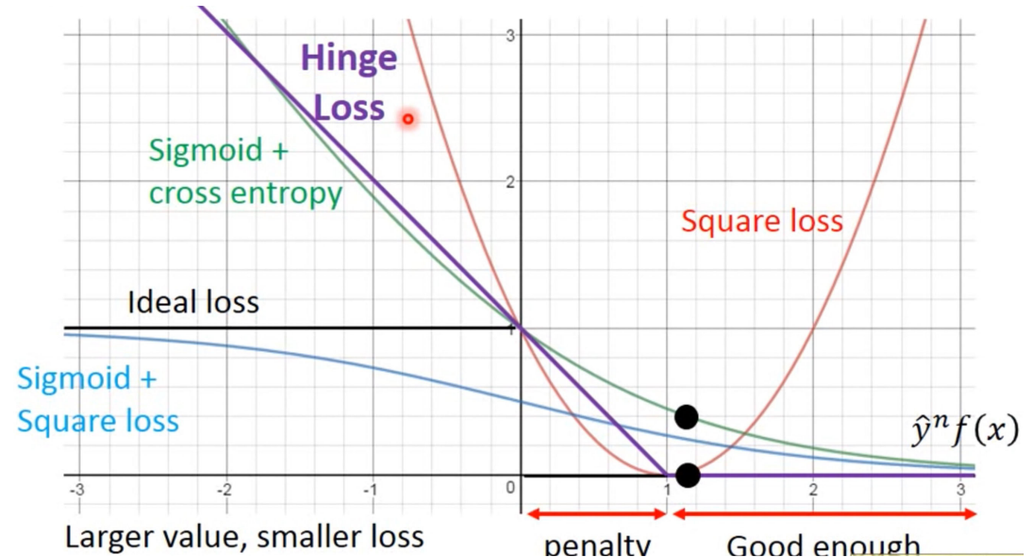

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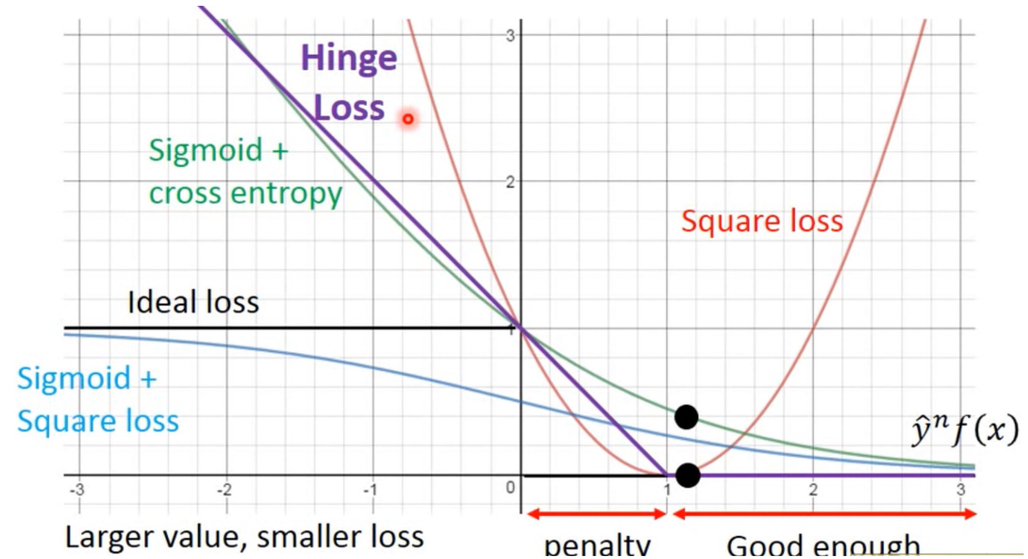

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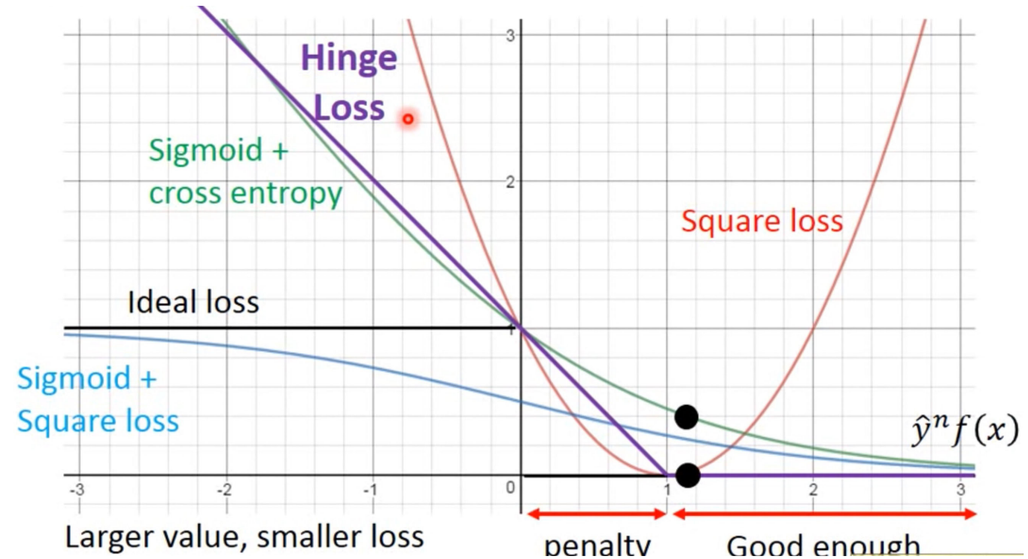

Hinge Loss.

$$l(f(x_i), y_i) = \max(0, 1 - y_i f(x_i))$$

- It achieves

$$f(x_i) = \begin{cases} \geq 1 & \text{when } y_i = 1 \\ \leq -1 & \text{when } y_i = -1 \end{cases}$$

Loss Function

How to choose a differentiable function to approximate l^{0-1}?

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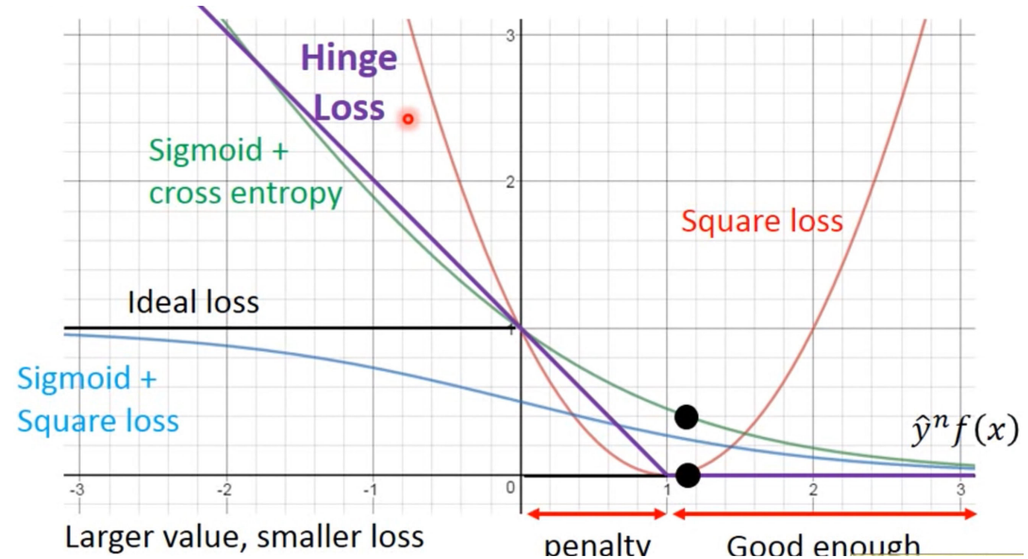

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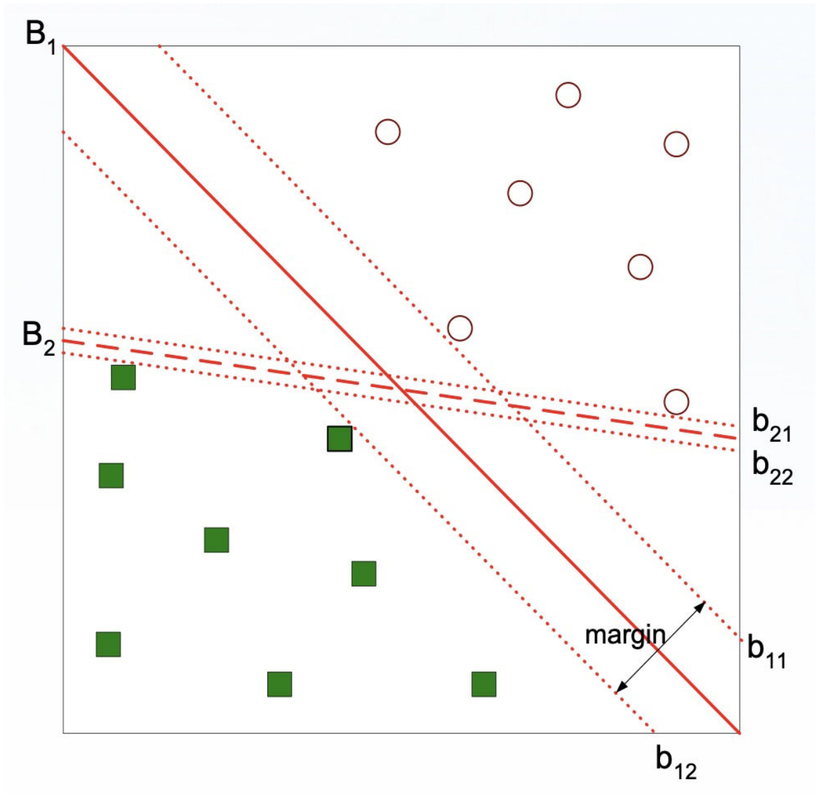
- It serves the purpose but different from *Sigmoid + Cross Entropy* loss.

Margin

Which separating hyperplane is better?



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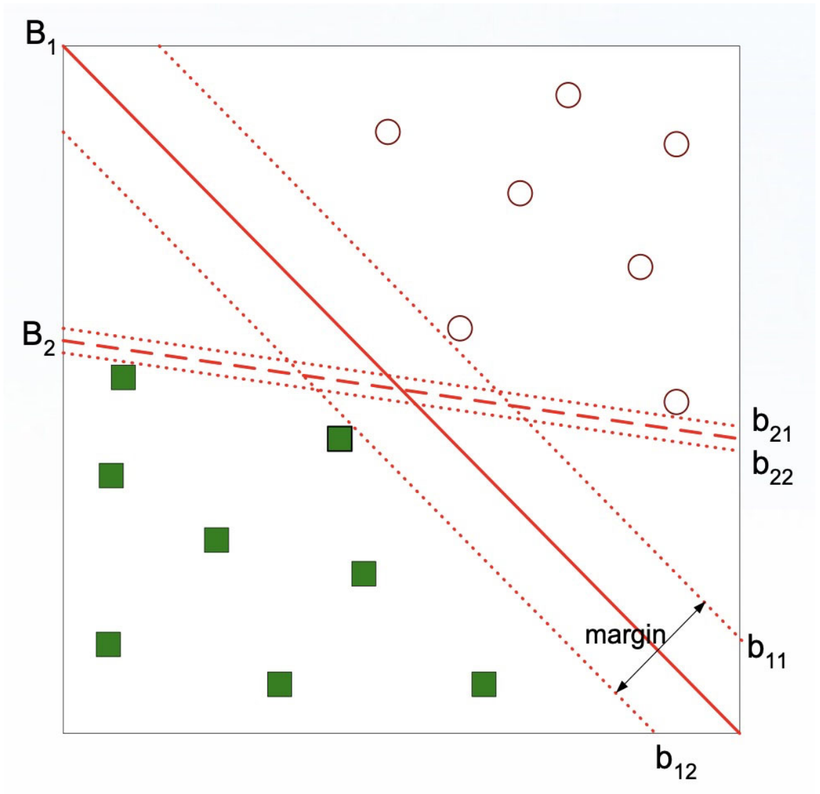

- Intuitively, solid red line is better.

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Given hyperplane defined by $L = \{v : \langle \omega, v \rangle + b = 0\}$ and give a point x, the distance of x to L is

$$d(x, L) = \min \|x - v\| : v \in L$$

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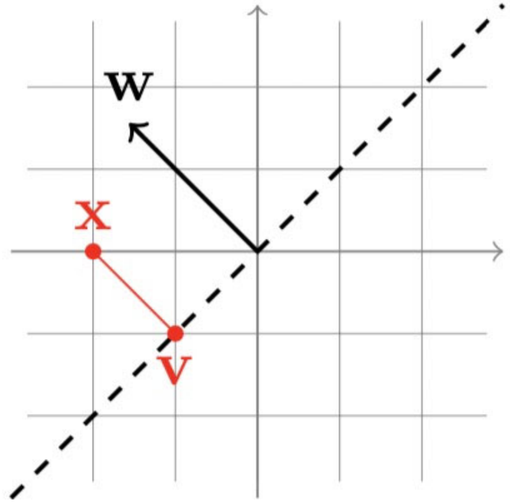

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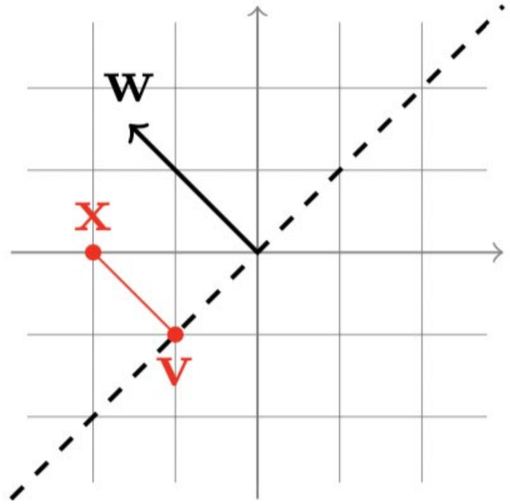

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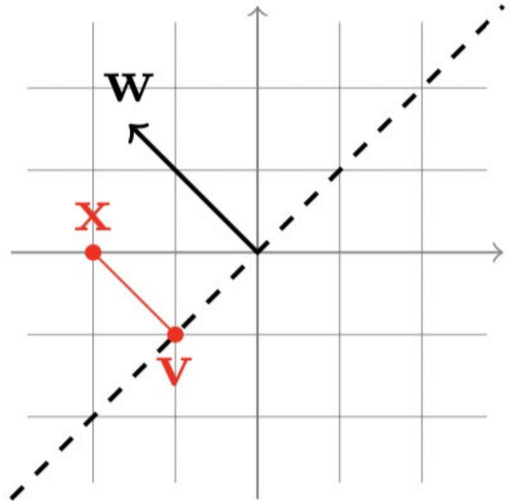

- Proof can be done easily.
- Some observation on the inner product: $\langle \omega, x \rangle = \|\omega\| \cdot \|x\| \cdot cos(\theta)$

Support Vector Machine (Hard-SVM)

When the sample is linearly separable, we seek for the separating hyperplane with largest margin $\operatorname{argmax}_{(\omega,b):\|\omega\|=1} \min_{i\in m} |\langle \omega, x_i\rangle + b|$, subject to $\forall i,\ y_i(\langle \omega, x_i\rangle + b) > 0$.

- equivalent to $\operatorname{argmax}_{(\omega,b):\|\omega\|=1} \min_{i\in m} y_i(\langle \omega, x_i\rangle + b)$
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Notes.

Margin is Scale Sensitive The margin depends on the scale of the examples

- if (ω, b) separates $(x_1, y_1), \ldots, (x_m, y_m)$ with margin γ, then it separates $(2x_1, y_1), \ldots, (2x_m, y_m)$ with a margin of 2γ

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Margin of distribution We say that $\mathscr{D}$ is separable with a (γ, ρ)-margin if exists (ω^*, b^*) s.t. $\|\omega^*\| = 1$ and $\mathscr{D}(\{(x, y) : \|x\| \leq \rho \bigwedge y(\langle \omega^*, x\rangle + b^*) \geq \gamma\}) = 1$

- then its sample complexity is $m(\epsilon, \delta) \leq \frac{8}{\epsilon^2} 2(\rho/\gamma)^2 + \log(2/\delta)$
- unlike the VC bounds, here the sample complexity depends on ρ/γ rather than d.

□

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$$\underset{(\omega,b):\|\omega\|=1}{\operatorname{argmin}} L(\omega,S) = \sum_{i=1}^{m} l(f(x_i),y_i) + \lambda\|\omega\|^2 = \sum_{i=1}^{m} \epsilon_i + \lambda\|\omega\|^2$$

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- This is the popular SVM formulation, which can be solved by *quadratic programming*.
- As an optimization problem, it can also be solved by *gradient descendant*.

□

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- Take partial derivatives to each component ω_j:

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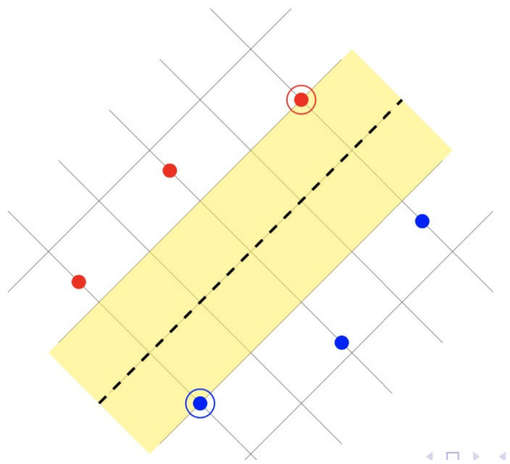
- For ω_j, the gradient descendant updating rule is $\omega_j = \omega_j - \eta \sum C_i(\omega_j)(x_j)_i$, in the vector form: $\omega = \omega - \eta \sum C_i(\omega)x_i$.

Support Vectors

A separating hyperplane is defined by (ω, b) subject to: $\forall i,\ y_i(\langle \omega, x_i \rangle + b) > 0$. The margin of a separating hyperplane is the distance of the closest example to it:

$$\min_i \| \langle \omega, x_i \rangle + b \|$$

Those closest examples are called support vectors.



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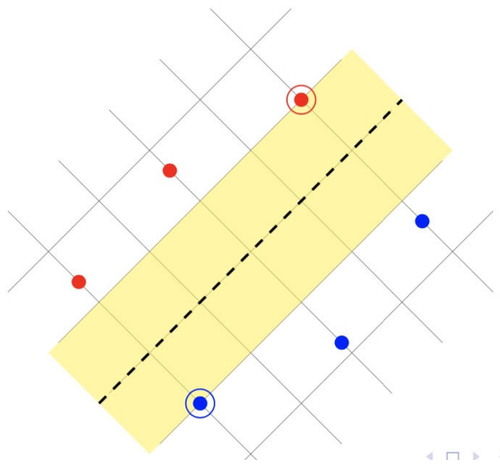

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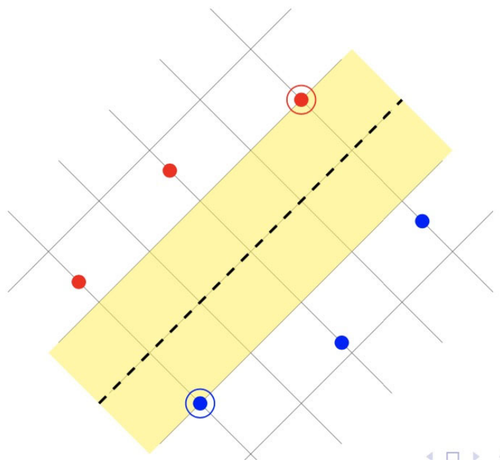

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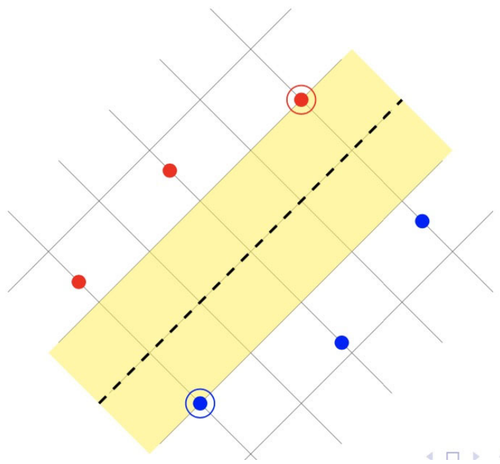

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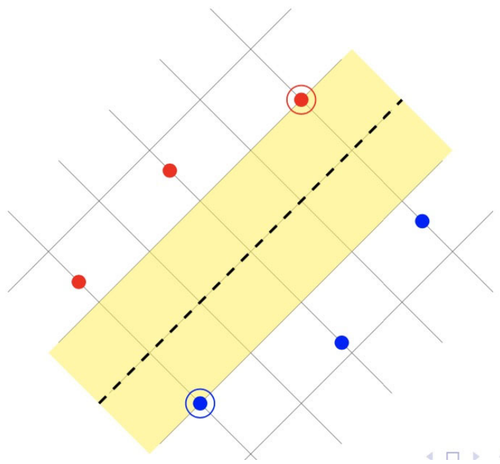

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- α^* may be sparse, and those x_i with non-zero α_i^* are support vectors.
  - For *Hinge loss*, α^* is usually sparse.
  - For *logistic regression* or *cross entropy*, α^* is usually non-zero.

Representer Theorem

Assume that ψ is a mapping from $\mathcal{X}$ to a Hilbert space (a feature space), then the SVM optimization is an instance of the following problem:

$$\underset{\omega}{\operatorname{argmin}}(f(\langle\omega,\psi(x_1)\rangle,\ldots,\langle\omega,\psi(x_m)\rangle)+R(\|\omega\|))$$

where $f:\mathcal{R}^m\mapsto\mathcal{R}$ is an arbitrary function. $R:\mathcal{R}_+\mapsto\mathcal{R}$ is a monotonically no-decreasing function, such as $\lambda\|\omega\|^2$. Then $\exists\alpha\in\mathcal{R}^m$ such that $\omega^*=\sum_{i=1}^m\alpha_i\psi(x_i)$.

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- Because ω^* is an element of a Hilbert space, so $\omega^*=\sum_{i=1}^m\alpha_i\psi(x_i)+u$, where $u\perp\psi(x_i)$ $\forall x_i$.

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- Hence the objective at ω equals the objective at ω^* minus $\lambda\alpha$. By optimality of ω^*, u must be zero.

□

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Implications.

- By representer theorem, the optimal solution can be written as $\omega^*=\sum_{i=1}^m\alpha_i\psi(x_i)$
- Denote by $\mathcal{G}$ the Gram matrix s.t. $\mathcal{G}_{i,j}=\langle\psi(x_i),\psi(x_j)\rangle$, we have:

$$\langle\omega,\psi(x_i)\rangle=\langle\sum_{i=1}^m\alpha_i\psi(x_i),\psi(x_i)\rangle=\sum_{i=1}^m\alpha_i\langle\psi(x_i),\psi(x_i)\rangle=(\mathcal{G}\alpha)_i,\quad\forall i$$

- Also $\|\omega\|^2=\alpha^T\mathcal{G}\alpha$. Hence, the optimisation task can be written as:

$$\operatorname*{argmin}_{\alpha\in\mathcal{R}^m}(f(\mathcal{G}\alpha)+\lambda\alpha^T\mathcal{G}\alpha)$$

Kernel Trick

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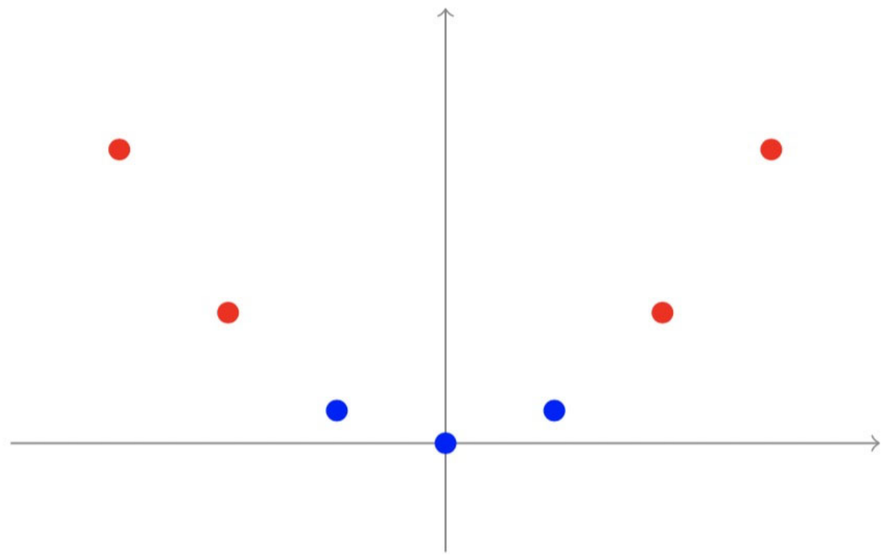
- It is separable in $\mathscr{R}^2$ by half-spaces if we may $x \mapsto (x, x^2)$



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- Observe that calculating $\mathcal{K}(x,y)$ takes $O(n)$ time while the dimension of $\psi(x)$ is nk

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- $\mathcal{K}(x,y) =< \psi(x), \psi(y) >= \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix} = x_1^2y_1^2 + 2x_1x_2y_1y_2 + x_2^2y_2^2 = (x \cdot y)^2$

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- Let the original instance space be R and consider the mapping ρ where for each non-negative integer $n \geq 0$ there exists an element $\psi_n(x)$ which equals to $\frac{1}{\sqrt{n!}} e^{-\frac{x^2}{2\delta}} x^n$.

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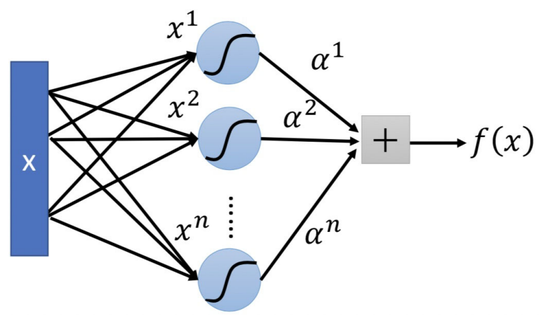

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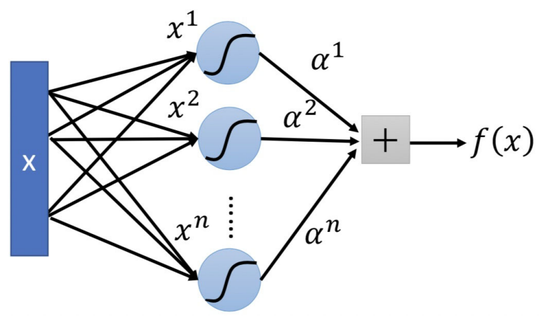

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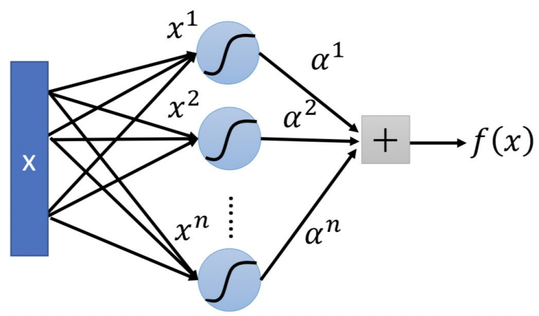

- The weight of each neuron is an example x_i.
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A symmetric function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \mapsto \mathcal{R}$ implements an inner product in some Hilbert space if and only if it is positive semi-definite; namely $\forall v_i$, the Gram matrix, $\mathcal{G}(i,j) = \mathcal{K}(x_i, x_j)$, is a positive semidefinite matrix.

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- It can be learned or designed by prior knowledge.

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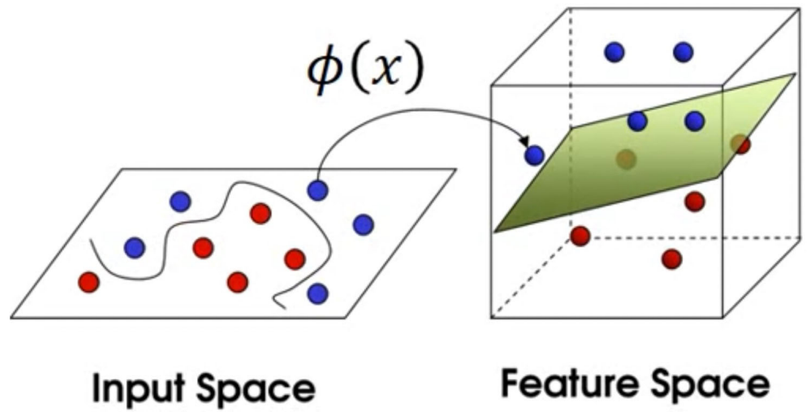
From Machine Learning to Deep Learning

Notes.

- SVM is a feature mapping followed by linear classifier (half-space): SVM kernel is learnable, but not as perfectly done as in ANN.



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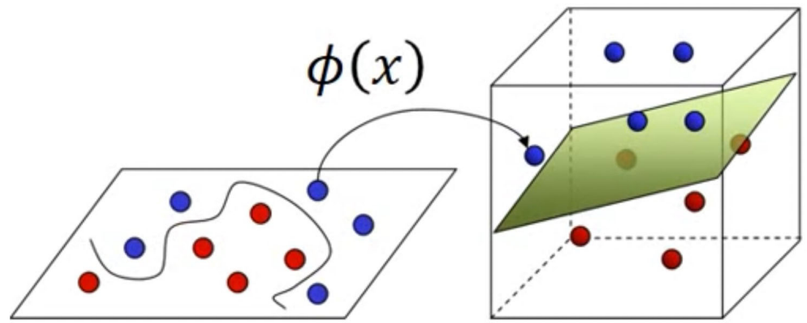
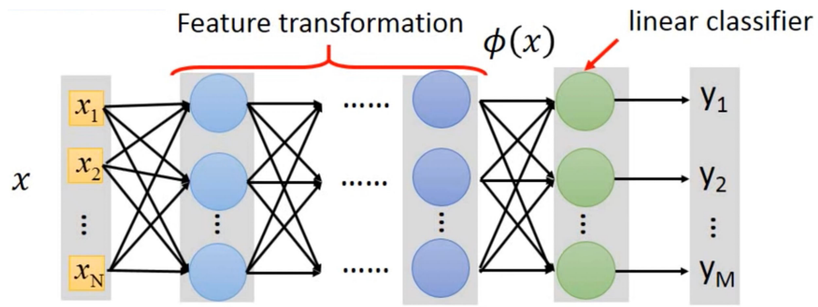


- Deep learning is feature transformations + linear classifier (half-space).



Quiz

SGD with Projection Step

A supermarket manager would like to learn which of his customers have babies on the basis of their shopping carts. Specifically, he sampled i.i.d. customers, where for customer i, let $x_i \subset \{1,\ldots,d\}$ denote the subset of items the customer bought, and let $y_i \in \{1,-1\}$ be the label indicating whether this customer has a baby. As prior knowledge, the manager knows that there are k items such that the label is determined to be 1 iff the customer bought at least one of these k items. Of course, the identity of these k items is not known (otherwise, there was nothing to learn). In addition, according to the store regulation, each customer can buy at most s items.

- Help the manager to design a learning algorithm such that both its time complexity and its sample complexity are polynomial in s, k, and $\frac{1}{\epsilon}$.

Questions?

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