Controling Complexity: Regularization

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(Slides credit to David Rosenberg, He He, et al.)

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Lecture Slides

- For those of you who want to take notes on your tablets.
- Otherwise, slides will be shared on the course website after the lecture.

Logistic Regression

- If the label is 0 or 1:
- $\hat{y} = \sigma(z)$, where σ is the sigmoid function.

$$\sigma(z) = \frac{1}{1 + \exp(-z)}.$$

- The loss is binary cross entropy:

$$\ell_{\text{Logistic}} = -y \log(\hat{y}) - (1-y) \log(1-\hat{y}).$$

- Remember the negative sign!

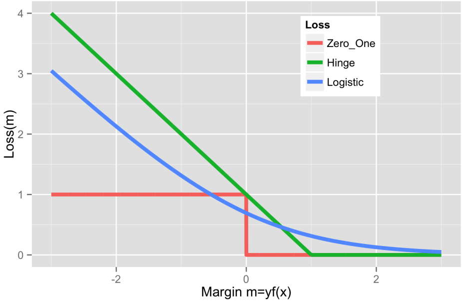
Logistic Regression

- If the label is -1 o 1:
- Note: $1 - \sigma(z) = \sigma(-z)$
- Now we can derive an equivalent loss form:

$$
\begin{aligned}
\ell_{\text{Logistic}} &= \begin{cases} -\log(\sigma(z)) & \text{if} \quad y = 1 \\ -\log(\sigma(-z)) & \text{if} \quad y = -1 \end{cases} \\
&= -\log(\sigma(yz)) \\
&= -\log(\frac{1}{1 + e^{-yz}}) \\
&= \log(1 + e^{-m}).
\end{aligned}
$$

Logistic Loss

Logistic/Log loss: $\ell_{\text{Logistic}} = \log\left(1 + e^{-m}\right)$



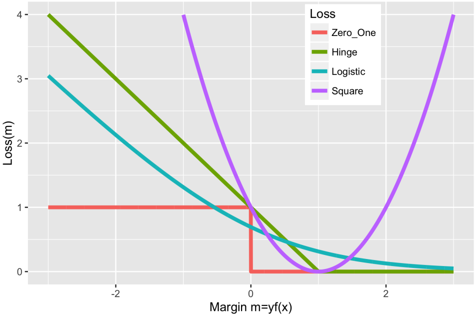
Logistic loss is differentiable. Logistic loss always rewards a larger margin (the loss is never 0).

What About Square Loss for Classification?

- Loss $\ell(f(x),y) = (f(x)-y)^2$.
- Turns out, can write this in terms of margin $m = f(x)y$:
- Using fact that $y^2 = 1$, since $y \in \{-1,1\}$.

$$
\begin{aligned}
\ell(f(x),y) &= (f(x)-y)^2 \\
&= f^2(x) - 2f(x)y + y^2 \\
&= f^2(x)y^2 - 2f(x)y + 1 \\
&= (1-f(x)y)^2 \\
&= (1-m)^2
\end{aligned}
$$

What About Square Loss for Classification?



Heavily penalizes outliers (e.g. mislabeled examples).

Complexity of Hypothesis Spaces

What is the trade-off between approximation error and estimation error?

- Bigger $\mathcal{F}$: better approximation but can overfit (need more samples)
- Smaller $\mathcal{F}$: less likely to overfit but can be farther from the true function

To control the "size" of $\mathcal{F}$, we need some measure of its complexity:

- Number of variables / features
- Degree of polynomial

General Approach to Control Complexity

1. Learn a sequence of models varying in complexity from the training data

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$$

   Example: Polynomial Functions

   - $\mathcal{F} = \{\text{all polynomial functions}\}$
   - $\mathcal{F}_d = \{\text{all polynomials of degree } \leqslant d\}$

2. Select one of these models based on a score (e.g. validation error)

Feature Selection in Linear Regression

Nested sequence of hypothesis spaces: $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_n \cdots \subset \mathcal{F}$

- $\mathcal{F} = \{$linear functions using all features$\}$
- $\mathcal{F}_d = \{$linear functions using fewer than d features$\}$

Best subset selection:

- Choose the subset of features that is best according to the score (e.g. validation error)
  - Example with two features: Train models using $\{\}$, $\{X_1\}$, $\{X_2\}$, $\{X_1, X_2\}$, respectively
- Not an efficient search algorithm; iterating over all subsets becomes very expensive with a large number of features

Greedy Selection Methods

Forward selection:

1. Start with an empty set of features S
2. For each feature i not in S
   - Learn a model using features $S \cup i$
   - Compute score of the model: α_i
3. Find the candidate feature with the highest score: $j = \arg\max_i \alpha_i$
4. If α_j improves the current best score, add feature j: $S \leftarrow S \cup j$ and go to step 2; return S otherwise.

Backward Selection:

- Start with all features; in each iteration, remove the worst feature

Feature Selection: Discussion

- Number of features as a measure of the complexity of a linear prediction function
- General approach to feature selection:
  - Define a score that balances training error and complexity
  - Find the subset of features that maximizes the score
- Forward & backward selection do not guarantee to find the best solution.
- Forward & backward selection do not in general result in the same subset.
- Could there be a more consistent way of formulating feature selection as an optimization problem?

ℓ_2 and ℓ_1 Regularization

Complexity Penalty

An objective that balances number of features and prediction performance:

$$\text{score}(S) = \text{training\_loss}(S) + \lambda|S| \tag{1}$$

λ balances the training loss and the number of features used.

- Adding an extra feature must be justified by at least λ improvement in training loss
- Larger $\lambda \rightarrow$ complex models are penalized more heavily

Complexity Penalty

Goal: Balance the complexity of the hypothesis space $\mathcal{F}$ and the training loss

Complexity measure: $\Omega : \mathcal{F} \to [0, \infty)$, e.g. number of features

Penalized ERM (Tikhonov regularization)

For complexity measure $\Omega : \mathcal{F} \to [0, \infty)$ and fixed $\lambda \geqslant 0$,

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

As usual, we find λ using the validation data.

Number of features as complexity measure is not differentiable and hard to optimize—other measures?

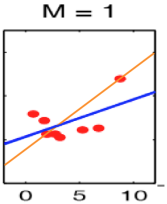
Soft Selection

- We can imagine having a weight for each feature dimension.
- In linear regression, the model weights multiply each feature dimension:

$$f(x) = w^\top x$$

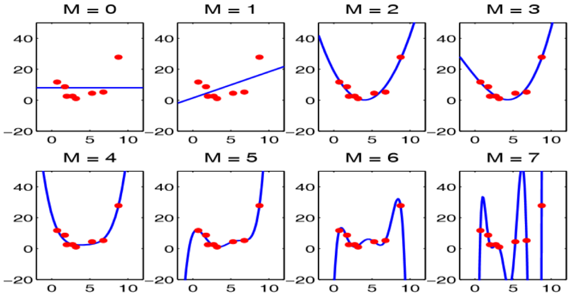
- If w_i is zero or close to zero, then it means that we are not using the i-th feature.

Weight Shrinkage: Intuition



- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?
- More stable: small change in the input does not cause large change in the output
- If we push the estimated weights to be small, re-estimating them on a new dataset wouldn't cause the prediction function to change dramatically (less sensitive to noise in data)

Weight Shrinkage: Polynomial Regression



- n-th feature dimension is the n-th power of x: $1, x, x^2, \ldots$
- Large weights are needed to make the curve wiggle sufficiently to overfit the data
- $\hat{y} = 0.001x^7 + 0.003x^3 + 1$ less likely to overfit than $\hat{y} = 1000x^7 + 500x^3 + 1$

(Adapated from Mark Schmidt's slide)

Linear Regression with ℓ_2 Regularization

- We have a linear model

$$\mathcal{F} = \left\{ f : \mathrm{R}^d \to \mathrm{R} \mid f(x) = w^T x \text{ for } w \in \mathrm{R}^d \right\}$$

- Square loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- Training data $\mathcal{D}_n = \left((x_1, y_1), \ldots, (x_n, y_n)\right)$
- Linear least squares regression is ERM for square loss over $\mathcal{F}$:

$$\hat{w} = \underset{w \in \mathrm{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$$

- This often overfits, especially when d is large compared to n (e.g. in NLP one can have 1M features for 10K documents).

Linear Regression with L2 Regularization

Penalizes large weights:

$$\hat{w} = \arg\min_{w \in \mathrm{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_2^2,$$

where $\|w\|_2^2 = w_1^2 + \cdots + w_d^2$ is the square of the ℓ_2-norm.

- Also known as **ridge regression**.
- Equivalent to linear least square regression when $\lambda = 0$.
- ℓ_2 regularization can be used for other models too (e.g. neural networks).

ℓ_2 regularization reduces sensitivity to changes in input

- $\hat{f}(x) = \hat{w}^T x$ is **Lipschitz continuous** with Lipschitz constant $L = \|\hat{w}\|_2$: when moving from x to $x+h$, $\hat{f}$ changes no more than $L\|h\|$.
- ℓ_2 regularization controls the maximum rate of change of $\hat{f}$.
- Proof:

$$\begin{aligned} \left|\hat{f}(x+h) - \hat{f}(x)\right| &= |\hat{w}^T(x+h) - \hat{w}^T x| = \left|\hat{w}^T h\right| \\ &\leqslant \|\hat{w}\|_2 \|h\|_2 \quad \text{(Cauchy-Schwarz inequality)} \end{aligned}$$

- Other norms also provide a bound on L due to the equivalence of norms: $\exists C > 0$ s.t. $\|\hat{w}\|_2 \leqslant C\|\hat{w}\|_p$

Linear Regression vs. Ridge Regression

Objective:

- Linear: $L(w) = \frac{1}{2}\|Xw - y\|_2^2$
- Ridge: $L(w) = \frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$

Gradient:

- Linear: $\nabla L(w) = X^T(Xw - y)$
- Ridge: $\nabla L(w) = X^T(Xw - y) + \lambda w$
  - Also known as **weight decay** in neural networks

Closed-form solution:

- Linear: $X^T Xw = X^T y$ -> $w = (X^T X)^{-1} X^T y$
- Ridge: $(X^T X + \lambda I)w = X^T y$ -> $w = (X^T X + \lambda I)^{-1} X^T y$
  - $(X^T X + \lambda I)$ is always invertible

Constrained Optimization

- L2 regularizer is a term in our optimization objective.

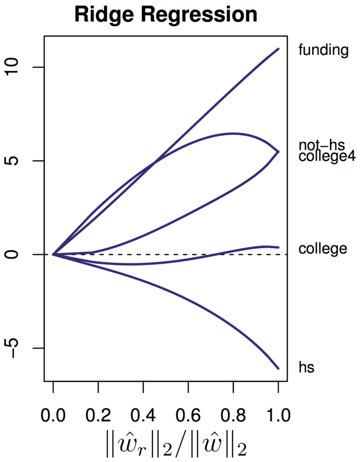
$$w^* = \arg\min_w \frac{1}{2}\|Xw - y\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$$

- This is also called the **Tikhonov** form.
- The Lagrangian theory allows us to interpret the second term as a constraint.

$$w^* = \arg\min_{w:\|w\|_2^2 \leqslant r} \frac{1}{2}\|Xw - y\|_2^2$$

- At optimum, the gradients of the main objective and the constraint cancel out.
- This is also called the **Ivanov** form.

Ridge Regression: Regularization Path



$$
\begin{aligned}
\hat{w}_r &= \underset{\|w\|_2^2 \le r^2}{\arg\min} \frac{1}{n}\sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2 \\
\hat{w} &= \hat{w}_\infty = \text{Unconstrained ERM}
\end{aligned}
$$

- For $r = 0$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 0$.
- For $r = \infty$, $\|\hat{w}_r\|_2/\|\hat{w}\|_2 = 1$

Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

Lasso Regression

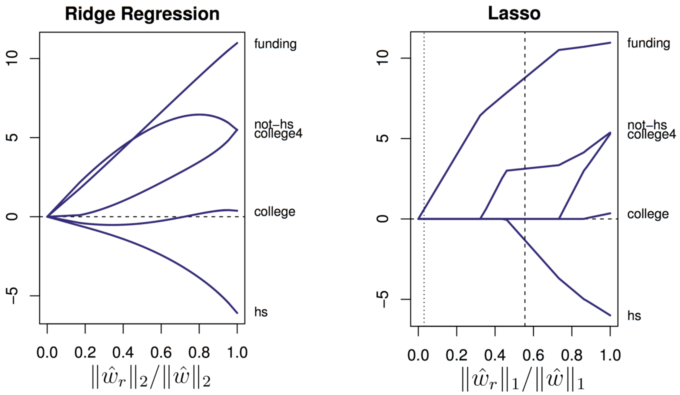
Penalize the ℓ_1 norm of the weights:

Lasso Regression (Tikhonov Form, soft penalty)

$$\hat{w} = \underset{w \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_1,$$

where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

Ridge vs. Lasso: Regularization Paths



Lasso yields sparse weights.

Modified from Hastie, Tibshirani, and Wainwright's *Statistical Learning with Sparsity*, Fig 2.1. About predicting crime in 50 US cities.

The Benefits of Sparsity

The coefficient for a feature is 0 $\implies$ the feature is not needed for prediction. Why is that useful?

- Faster to compute the features; cheaper to measure or annotate them
- Less memory to store features (deployment on a mobile device)
- Interpretability: identifies the important features
- Prediction function may generalize better (model is less complex)

Why does ℓ_1 Regularization Lead to Sparsity?

Lasso Regression

Penalize the ℓ_1 norm of the weights:

Lasso Regression (Tikhonov Form, soft penalty)

$$\hat{w} = \underset{w \in \mathrm{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda \|w\|_1,$$

where $\|w\|_1 = |w_1| + \cdots + |w_d|$ is the ℓ_1-norm.

Regularization as Constrained ERM

Constrained ERM (Ivanov regularization)

For complexity measure $\Omega : \mathcal{F} \to [0, \infty)$ and fixed $r \geqslant 0$,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

$$\text{s.t. } \Omega(f) \leqslant r$$

Lasso Regression (Ivanov Form, hard constraint)

The lasso regression solution for complexity parameter $r \geqslant 0$ is

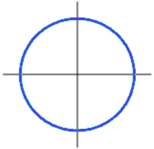
$$\hat{w} = \operatorname*{arg\,min}_{\|w\|_1 \leqslant r} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 .$$

r has the same role as λ in penalized ERM (Tikhonov).

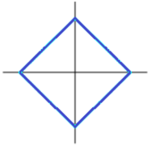
The ℓ_1 and ℓ_2 Norm Constraints

- Let's consider $\mathcal{F} = \{f(x) = w_1 x_1 + w_2 x_2\}$ space)
- We can represent each function in $\mathcal{F}$ as a point $(w_1, w_2) \in \mathrm{R}^2$.
- Where in R^2 are the functions that satisfy the Ivanov regularization constraint for ℓ_1 and ℓ_2?

  - ℓ_2 contour: $w_1^2 + w_2^2 = r$

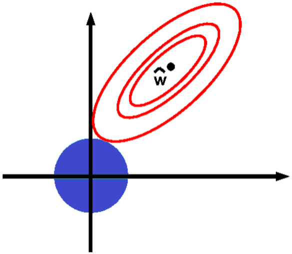


  - ℓ_1 contour: $|w_1| + |w_2| = r$



- Where are the sparse solutions?

- $f_r^* = \arg\min_{w \in \mathbb{R}^2} \sum_{i=1}^n \left(w^T x_i - y_i\right)^2$ subject to $w_1^2 + w_2^2 \leqslant r$

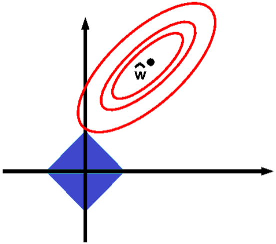


- Blue region: Area satisfying complexity constraint: $w_1^2 + w_2^2 \leqslant r$
- Red lines: contours of the empirical risk $\hat{R}_n(w) = \sum_{i=1}^n \left(w^T x_i - y_i\right)^2$.

KPM Fig. 13.3

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

- $f_r^* = \arg\min_{w \in \mathbb{R}^2} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$ subject to $|w_1| + |w_2| \leqslant r$



- Blue region: Area satisfying complexity constraint: $|w_1| + |w_2| \leqslant r$
- Red lines: contours of the empirical risk $\hat{R}_n(w) = \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$.
- ℓ_1 solution tends to touch the corners.

KPM Fig. 13.3

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Suppose the loss contour is growing like a perfect circle/sphere.
Geometric intuition: Projection onto diamond encourages solutions at corners.

- $\hat{w}$ in red/green regions are closest to corners in the ℓ_1 "ball".

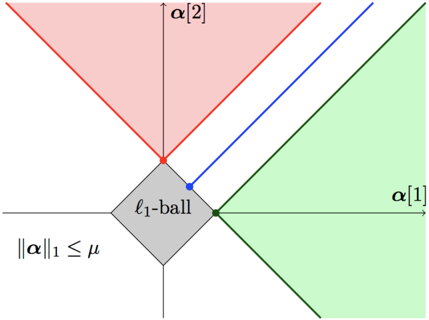


Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Suppose the loss contour is growing like a perfect circle/sphere.
Geometric intuition: Projection onto ℓ_2 sphere favors all directions equally.

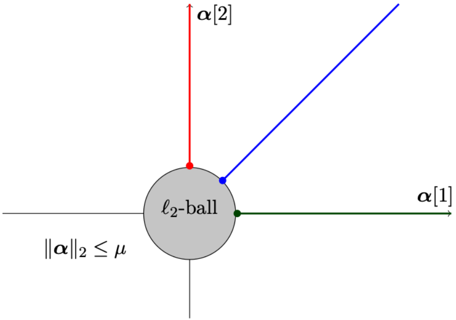


Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

Optimization Perspective

For ℓ_2 regularization,

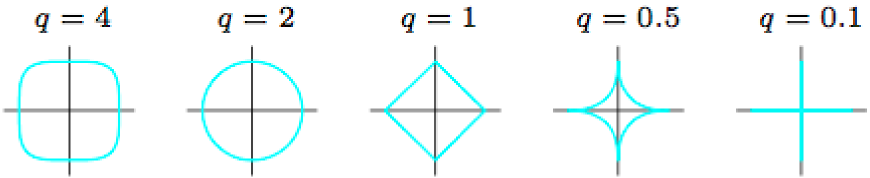
- As w_i becomes smaller, there is less and less penalty
  - What is the ℓ_2 penalty for $w_i = 0.0001$?
- The gradient—which determines the pace of optimization—decreases as w_i approaches zero
- Less incentive to make a small weight equal to exactly zero

For ℓ_1 regularization,

- The gradient stays the same as the weights approach zero
- This pushes the weights to be exactly zero even if they are already small

(ℓ_q) Regularization

- We can generalize to ℓ_q : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.

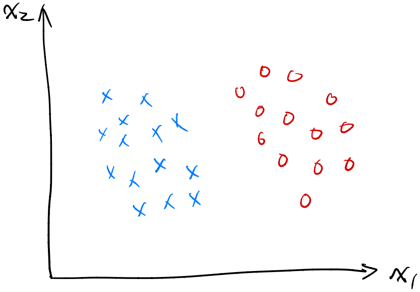


- Note: $\|w\|_q$ is only a norm if $q \geqslant 1$, but not for $q \in (0,1)$
- When $q < 1$, the ℓ_q constraint is non-convex, so it is hard to optimize; lasso is good enough in practice
- ℓ_0 ($\|w\|_0$) is defined as the number of non-zero weights, i.e. subset selection

Maximum Margin Classifier

Linearly Separable Data

Consider a linearly separable dataset $\mathcal{D}$:

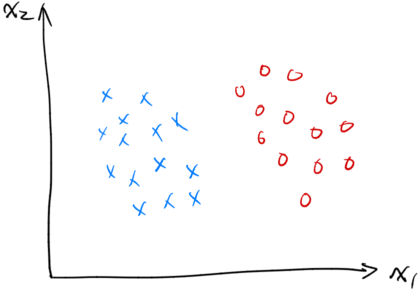


Find a separating hyperplane such that

- $w^T x_i > 0$ for all x_i where $y_i = +1$
- $w^T x_i < 0$ for all x_i where $y_i = -1$

Linearly Separable Data

Consider a linearly separable dataset $\mathcal{D}$:



Now let's design a learning algorithm: If there is a misclassified example, change the hyperplane according to the example.

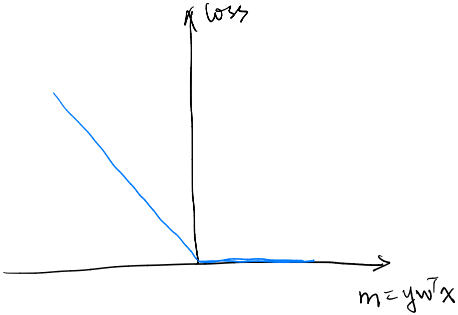
The Perceptron Algorithm

- Initialize $w \leftarrow 0$
- While not converged (exists misclassified examples)
  - For $(x_i, y_i) \in \mathcal{D}$
    - If $y_i w^T x_i < 0$ (wrong prediction)
    - Update $w \leftarrow w + y_i x_i$
- Intuition: move towards misclassified positive examples and away from negative examples
- Guarantees to find a zero-error classifier (if one exists) in finite steps
- What is the loss function if we consider this as a SGD algorithm?

Minimize the Hinge Loss

Perceptron Loss

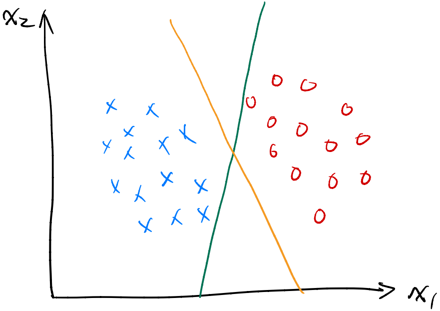
$$\ell(x, y, w) = \max(0, -yw^T x)$$



Maximum-Margin Separating Hyperplane

For separable data, there are infinitely many zero-error classifiers.

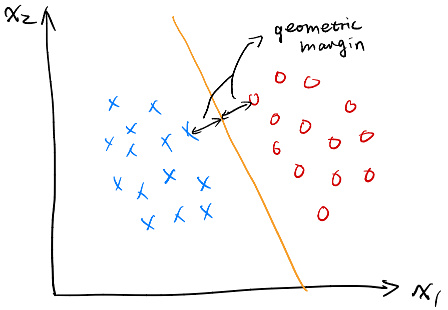
Which one do we pick?



(Perceptron does not return a unique solution.)

Maximum-Margin Separating Hyperplane

We prefer the classifier that is farthest from both classes of points



- Geometric margin: smallest distance between the hyperplane and the points
- Maximum margin: *largest* distance to the closest points

Geometric Margin

We want to maximize the distance between the separating hyperplane and the closest points.

Let's formalize the problem.

Definition (separating hyperplane)

We say (x_i, y_i) for $i = 1, \ldots, n$ are **linearly separable** if there is a $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that $y_i(w^T x_i + b) > 0$ for all i. The set $\{v \in \mathbb{R}^d \mid w^T v + b = 0\}$ is called a **separating hyperplane**.

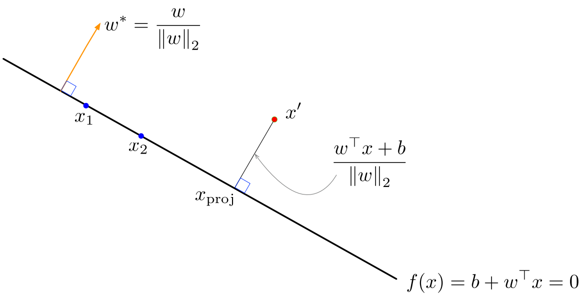
Definition (geometric margin)

Let H be a hyperplane that separates the data (x_i, y_i) for $i = 1, \ldots, n$. The **geometric margin** of this hyperplane is

$$\min_i d(x_i, H),$$

the distance from the hyperplane to the closest data point.

Distance between a Point and a Hyperplane



- Any point on the plane p, and normal vector $w/\|w\|_2$
- Projection of x onto the normal: $\frac{(x'-p)^T w}{\|w\|_2}$
- $(x'-p)^T w = x'^T w - p^T w = x'^T w + b$ (since $p^T w + b = 0$)
- Signed distance between x' and Hyperplane H: $\frac{w^T x' + b}{\|w\|_2}$
- Taking into account of the label y: $d(x', H) = \frac{y(w^T x' + b)}{\|w\|_2}$

Maximize the Margin

We want to maximize the geometric margin:

$$\text{maximize } \min_i d(x_i, H).$$

Given separating hyperplane $H = \left\{ v \mid w^T v + b = 0 \right\}$, we have

$$\text{maximize } \min_i \frac{y_i(w^T x_i + b)}{\|w\|_2}.$$

Let's remove the inner minimization problem by

$$\begin{array}{ll} \text{maximize} & M \\ \text{subject to} & \frac{y_i(w^T x_i + b)}{\|w\|_2} \geqslant M \quad \text{for all } i \end{array}$$

Note that the solution is not unique (why?).

Maximize the Margin

Let's fix the norm $\|w\|_2$ to $1/M$ to obtain:

$$\begin{array}{ll} \text{maximize} & \frac{1}{\|w\|_2} \\ \text{subject to} & y_i(w^T x_i + b) \geqslant 1 \quad \text{for all } i \end{array}$$

It's equivalent to solving the minimization problem

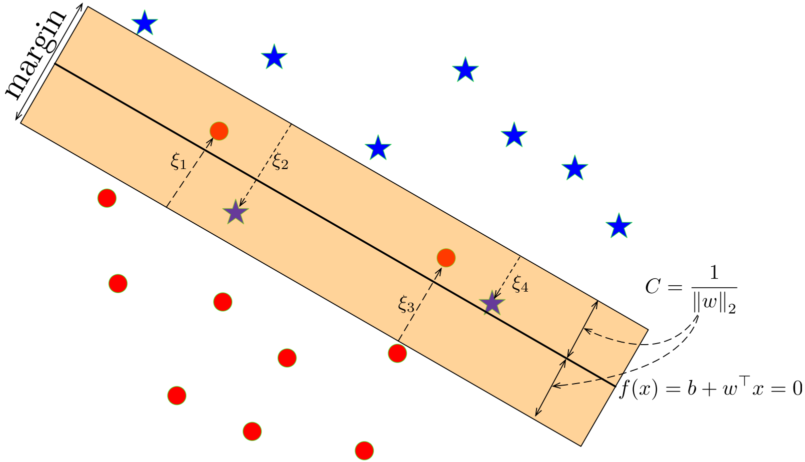
$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|_2^2 \\ \text{subject to} & y_i(w^T x_i + b) \geqslant 1 \quad \text{for all } i \end{array}$$

Note that $y_i(w^T x_i + b)$ is the (functional) margin. The optimization finds the minimum norm solution which has a margin of at least 1 on all examples.

Not linearly separable

What if the data is *not* linearly separable?

For any w, there will be points with a negative margin.



Soft Margin SVM

Introduce **slack variables** ξ's to penalize small margin:

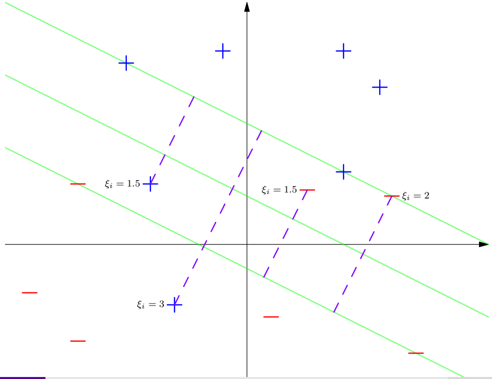
$$
\begin{aligned}
\text{minimize} \quad & \frac{1}{2}\|w\|_2^2 + \frac{C}{n}\sum_{i=1}^n \xi_i \\
\text{subject to} \quad & y_i(w^T x_i + b) \geqslant 1 - \xi_i \quad \text{for all } i \\
& \xi_i \geqslant 0 \quad \text{for all } i
\end{aligned}
$$

- If $\xi_i = 0 \; \forall i$, it's reduced to hard SVM.
- What does $\xi_i > 0$ mean?
- What does C control?

Slack Variables

$d(x_i, H) = \frac{y_i(w^T x_i + b)}{\|w\|_2} \geqslant \frac{1-\xi_i}{\|w\|_2}$, thus ξ_i measures the violation by multiples of the geometric margin:

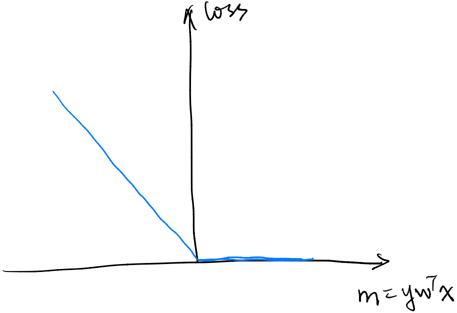
- $\xi_i = 1$: x_i lies on the hyperplane
- $\xi_i = 3$: x_i is past 2 margin width beyond the decision hyperplane



Minimize the Hinge Loss

Perceptron Loss

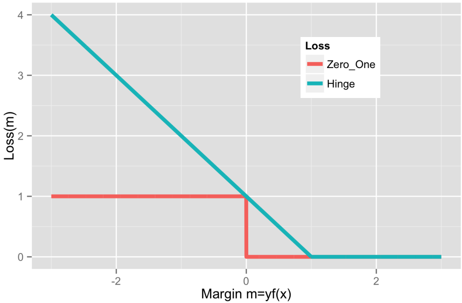
$$\ell(x, y, w) = \max(0, -yw^T x)$$



If we do ERM with this loss function, what happens?

Hinge Loss

- SVM/Hinge loss: $\ell_{\text{Hinge}} = \max\{1-m, 0\} = (1-m)_+$
- Margin $m = yf(x)$; "Positive part" $(x)_+ = x\mathbb{1}[x \geqslant 0]$.



Hinge is a **convex**, **upper bound** on $0-1$ loss. Not differentiable at $m=1$.
We have a **"margin error"** when $m<1$.