Controling Complexity: Feature Selection and Regularization

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

Feature Selection in Linear Regression

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

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- Not an efficient search algorithm; iterating over all subsets becomes very expensive with a large number of features

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Backward Selection:

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

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- 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:

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

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

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

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As usual, we find λ using the validation data.

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

Soft Selection

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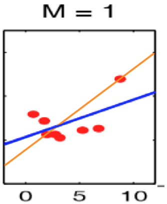
- If w_i is zero or close to zero, then it means that we are not using the i-th feature.

Weight Shrinkage: Intuition



- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?

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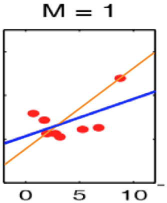

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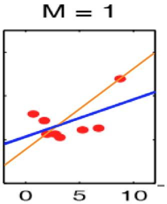
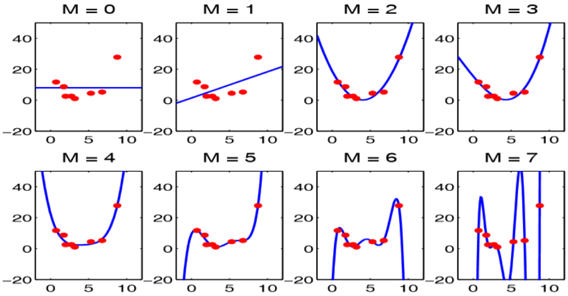


- Why would we prefer a regression line with smaller slope (unless the data strongly supports a larger slope)?

- 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



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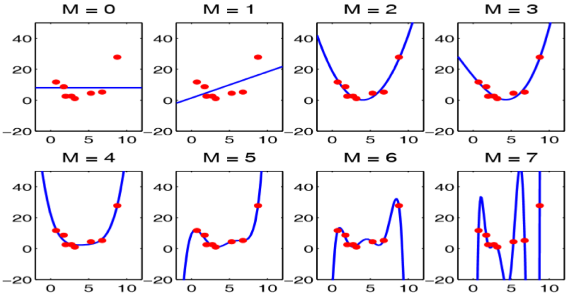

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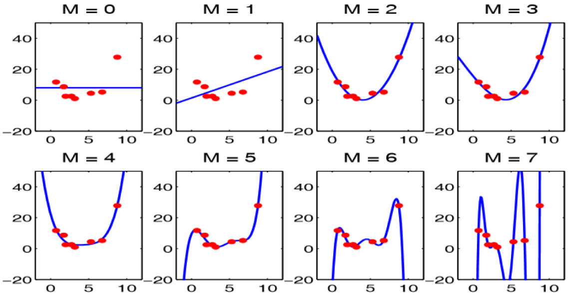

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- Large weights are needed to make the curve wiggle sufficiently to overfit the data
- $\hat{y} = 0.001x^7 + 0.003x^3 + 1$ less likely to overfit than $\hat{y} = 1000x^7 + 500x^3 + 1$

(Adapated from Mark Schmidt's slide)

Linear Regression with ℓ_2 Regularization

- We have a linear model

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

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

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

- 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:

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

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

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- 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 $L\|h\|$.

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

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Closed-form solution:

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- 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.

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

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- 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.

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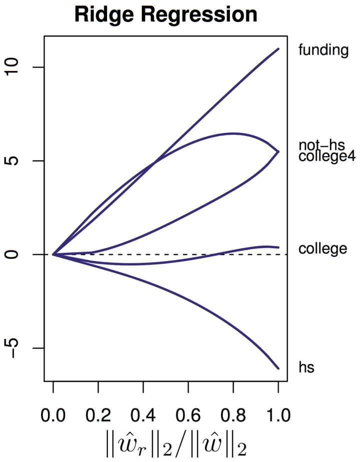
- The conditions for this equivalence can be derived from the Lagrangian theory.
- In practice, both approaches are effective: we will use whichever one is more convenient for training or analysis.

Ridge Regression: Regularization Path



$$\hat{w}_r = \underset{\|w\|_2^2 \le r^2}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$$

$$\hat{w} = \hat{w}_\infty = \text{Unconstrained ERM}$$

- 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)

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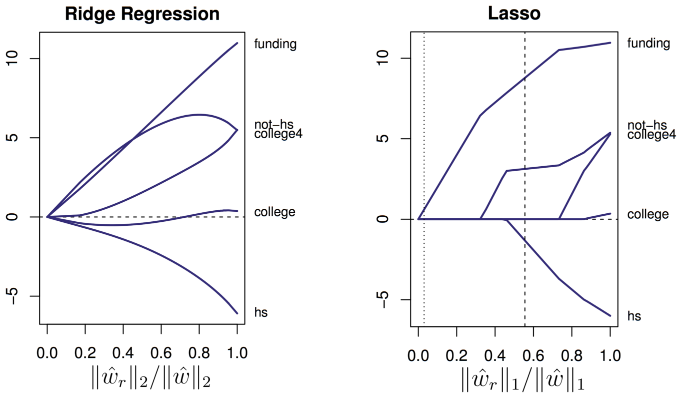
Ridge vs. Lasso: Regularization Paths



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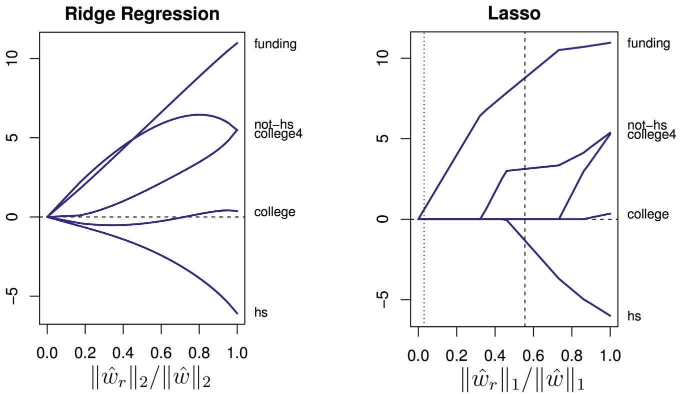

Lasso yields sparse weights.

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- Interpretability: identifies the important features
- Prediction function may generalize better (model is less complex)

Why does ℓ_1 Regularization Lead to Sparsity?

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Regularization as Constrained ERM

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

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 $\mathcal{F} = \{f(x) = w_1x_1 + w_2x_2\}$ 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?

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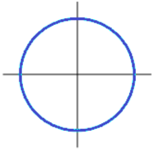
- ℓ_2 contour: $w_1^2 + w_2^2 = r$



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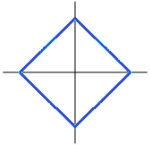

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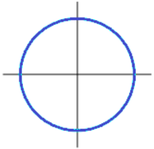

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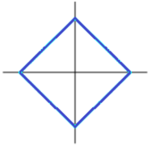
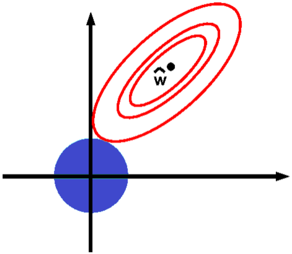


- Where are the sparse solutions?

Visualizing Regularization

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

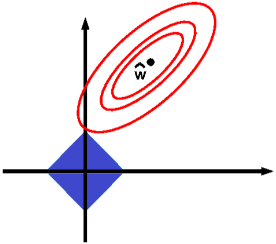


- Blue region: Area satisfying complexity constraint: $w_1^2 + w_2^2 \leqslant r$
- Red lines: contours of the empirical risk $\hat{R}_n(w) = \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2$.

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 $|w_1| + |w_2| \leqslant r$



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- ℓ_1 solution tends to touch the corners.

KPM Fig. 13.3

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Geometric intuition: Projection onto diamond encourages solutions at corners.

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

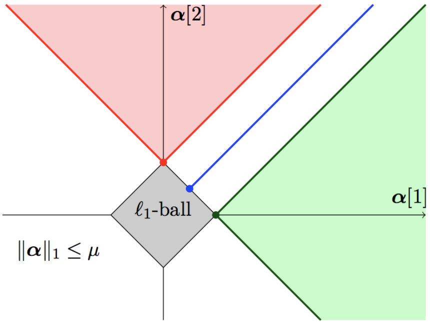
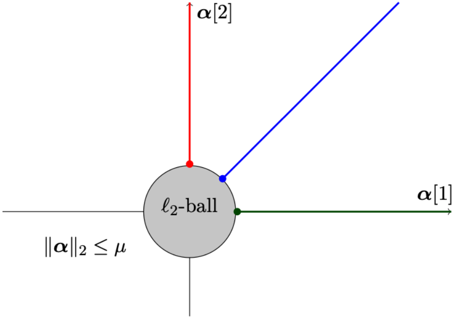


Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.6

Why Does ℓ_1 Regularization Encourage Sparse Solutions?

Geometric intuition: Projection onto ℓ_2 sphere favors all directions equally.



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Why does ℓ_2 Encourage Sparsity? 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

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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 : $(\|w\|_q)^q = |w_1|^q + |w_2|^q$.

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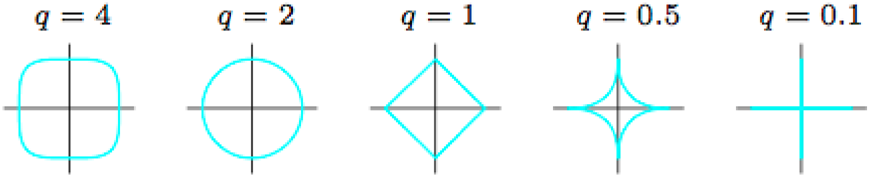

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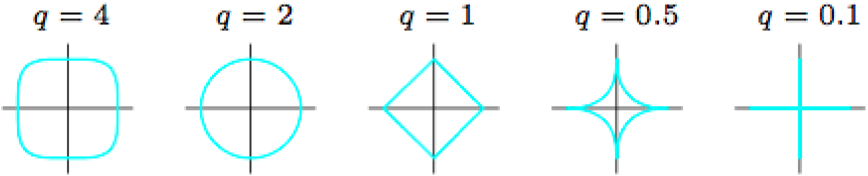

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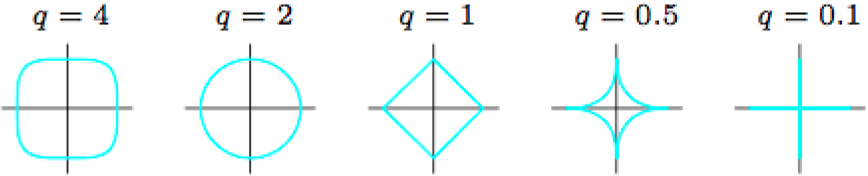

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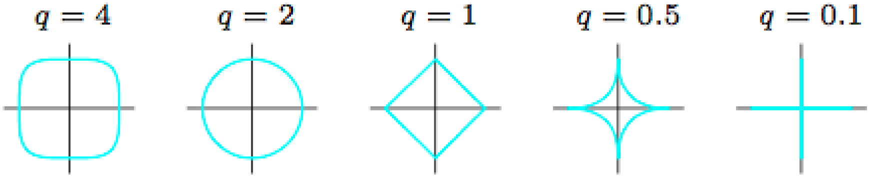

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- When $q < 1$, the ℓ_q constraint is non-convex, so it is hard to optimize; lasso is good enough in practice
- ℓ_0 ($\|w\|_0$) is defined as the number of non-zero weights, i.e. subset selection

Minimizing the lasso objective

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- The ridge regression objective is differentiable (and there is a closed form solution)
- Lasso objective function:

$$\min_{w \in \mathrm{R}^d} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda \|w\|_1$$

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- $\|w\|_1 = |w_1| + \ldots + |w_d|$ is not differentiable!
- We will briefly review three approaches for finding the minimum:
    - Quadratic programming
    - Projected SGD
    - Coordinate descent

Rewriting the Absolute Value

- Consider any number $a \in R$.
- Let the **positive part** of a be
$$a^+ = a\mathbb{1}[a \geqslant 0].$$
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- How do you write a in terms of a^+ and a^-?
- How do you write $|a|$ in terms of a^+ and a^-?

The Lasso as a Quadratic Program

Substituting $w = w^+ - w^-$ and $|w| = w^+ + w^-$ results in an equivalent problem:

$$\begin{array}{rl} \min_{w^+, w^-} & \sum_{i=1}^{n} \left(\left(w^+ - w^-\right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^-\right) \\ \text{subject to} & w_i^+ \geqslant 0 \text{ for all } i \quad \text{and} \quad w_i^- \geqslant 0 \text{ for all } i, \end{array}$$

- This objective is **differentiable** (in fact, **convex and quadratic**)

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- This objective is **differentiable** (in fact, **convex and quadratic**)
- How many variables does the new objective have?
- This is a **quadratic program**: a convex quadratic objective with linear constraints.
- Quadratic programming is a very well understood problem; we can plug this into a generic QP solver.

Are we missing some constraints?

We have claimed that the following objective is equivalent to the lasso problem:

$$\min_{w^+, w^-} \sum_{i=1}^{n} \left(\left(w^+ - w^- \right)^T x_i - y_i \right)^2 + \lambda 1^T \left(w^+ + w^- \right)$$

$$\text{subject to} \quad w_i^+ \geqslant 0 \text{ for all } i \qquad w_i^- \geqslant 0 \text{ for all } i,$$

- When we plug this optimization problem into a QP solver,
  - it just sees $2d$ variables and $2d$ constraints.
  - Doesn't know we want w_i^+ and w_i^- to be positive and negative parts of w_i.
- Turns out that these constraints will be satisfied anyway!
- To make it clear that the solver isn't aware of the constraints of w_i^+ and w_i^-, let's denote them a_i and b_i

The Lasso as a Quadratic Program

(Trivially) reformulating the lasso problem:

$$
\begin{aligned}
\min_{w} \min_{a,b} \quad & \sum_{i=1}^{n} \left((a-b)^T x_i - y_i \right)^2 + \lambda 1^T (a+b) \\
\text{subject to} \quad & a_i \geqslant 0 \text{ for all } i \qquad b_i \geqslant 0 \text{ for all } i, \\
& a-b = w \\
& a+b = |w|
\end{aligned}
$$

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& a + b = |w|
\end{aligned}$$

Claim: Don't need the constraint $a + b = |w|$.

Exercise: Prove by showing that the optimal solutions a^* and b^* satisfies $\min(a^*, b^*) = 0$, hence $a^* + b^* = |w|$.

The Lasso as a Quadratic Program

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& a - b = w
\end{aligned}
$$

Claim: Can remove $\min_w$ and the constraint $a - b = w$.

Exercise: Prove by switching the order of the minimization.

Projected SGD

- Now that we have a differentiable objective, we could also use gradient descent
- But how do we handle the constraints?

$$\min_{w^+,w^-\in\mathbb{R}^d} \sum_{i=1}^{n}\left(\left(w^+-w^-\right)^T x_i - y_i\right)^2 + \lambda 1^T\left(w^+ + w^-\right)$$
$$\text{subject to } w_i^+ \geqslant 0 \text{ for all } i$$
$$w_i^- \geqslant 0 \text{ for all } i$$

- Projected SGD is just like SGD, but after each step
  - We project w^+ and w^- into the constraint set.
  - In other words, if any component of w^+ or w^- becomes negative, we set it back to 0.

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots, w_d)$ over $w = (w_1, \ldots, w_d) \in \mathbf{R}^d$.

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Coordinate Descent Method

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- In gradient descent or SGD, each step potentially changes all entries of w.
- In **coordinate descent**, each step adjusts only a single coordinate w_i.

$$w_i^{\text{new}} = \underset{w_i}{\arg\min}\, L(w_1, \ldots, w_{i-1}, \mathrm{w_i}, w_{i+1}, \ldots, w_d)$$

- Solving the argmin for a particular coordinate may itself be an iterative process.
- Coordinate descent is an effective method when it's easy (or easier) to minimize w.r.t. one coordinate at a time

Coordinate Descent Method

Goal: Minimize $L(w) = L(w_1, \ldots w_d)$ over $w = (w_1, \ldots, w_d) \in \mathbf{R}^d$.

- **Initialize** $w^{(0)} = 0$
- **while** not converged:
  - Choose a coordinate $j \in \{1, \ldots, d\}$
  - $w_j^{\text{new}} \leftarrow \arg\min_{w_j} L(w_1^{(t)}, \ldots, w_{j-1}^{(t)}, \mathrm{w_j}, w_{j+1}^{(t)}, \ldots, w_d^{(t)})$
  - $w_j^{(t+1)} \leftarrow w_j^{\text{new}}$ and $w^{(t+1)} \leftarrow w^{(t)}$
  - $t \leftarrow t+1$

- Random coordinate choice $\implies$ **stochastic coordinate descent**
- Cyclic coordinate choice $\implies$ **cyclic coordinate descent**

Coordinate Descent Method for Lasso

The lasso objective coordinate minimization has a closed form! If

$$\hat{w}_j = \underset{w_j \in R}{\arg\min} \sum_{i=1}^{n} \left(w^T x_i - y_i\right)^2 + \lambda |w|_1$$

Then

$$\hat{w}_j = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

$$a_j = 2\sum_{i=1}^{n} x_{i,j}^2 \qquad c_j = 2\sum_{i=1}^{n} x_{i,j}(y_i - w_{-j}^T x_{i,-j})$$

where w_{-j} is w without the j-th component, and $x_{i,-j}$ is x_i without the j-th component.

Coordinate Descent in General

- In general, coordinate descent is not competitive with gradient descent: its convergence rate is slower and the iteration cost is similar

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Coordinate Descent in General

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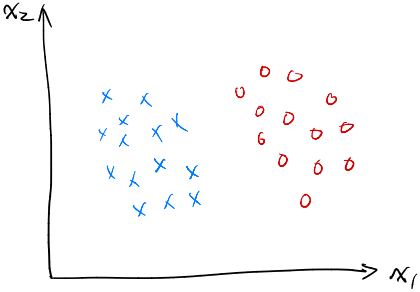
- But it works very well for certain problems
- Very simple and easy to implement
- Example applications: lasso regression, SVMs

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 $y_i = -1$

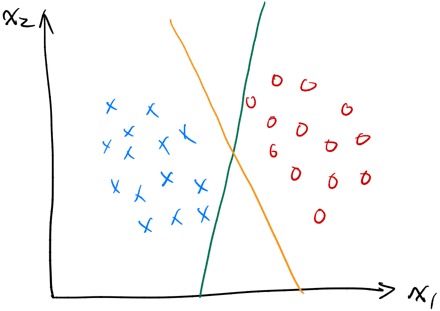
The Perceptron Algorithm

- 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?

Maximum-Margin Separating Hyperplane

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

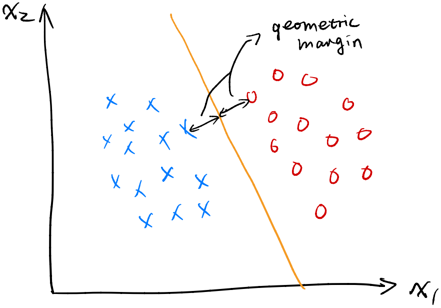
Which one do we pick?



(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**.

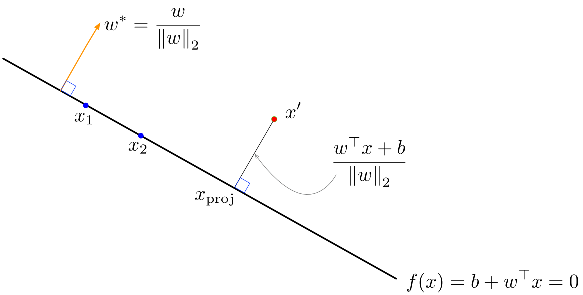
Definition (geometric margin)

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 $w/\|w\|_2$

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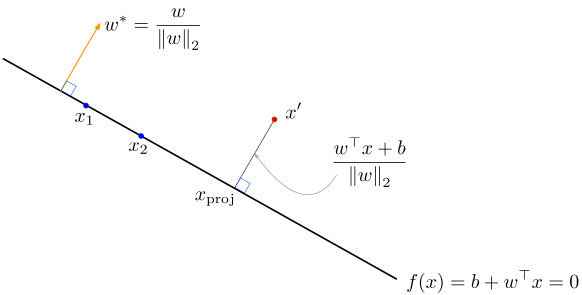

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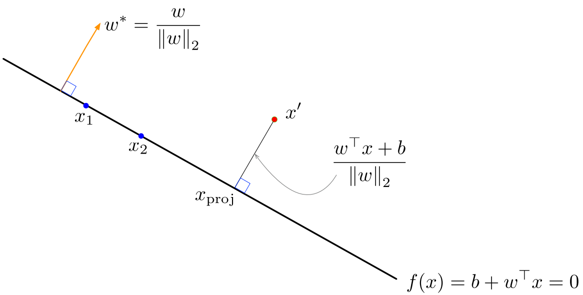

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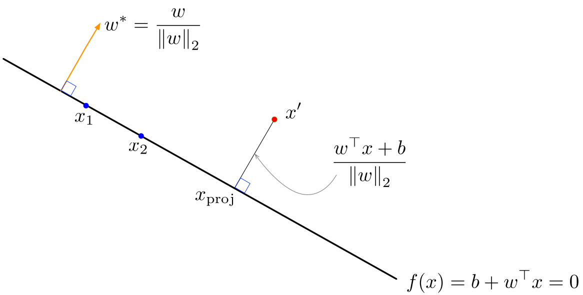

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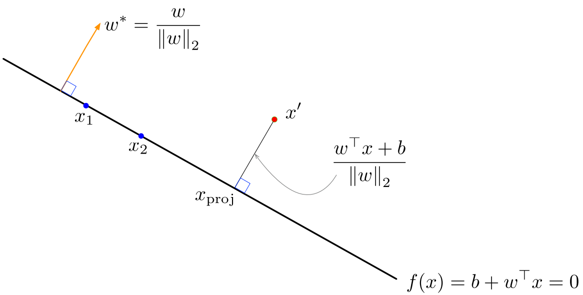
- $(x'-p)^T w = x'^T w - p^T w = x'^T w + b$ (since $p^T w + b = 0$)
- Signed distance between x' and Hyperplane H: $\frac{w^T x' + b}{\|w\|_2}$

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:

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Let's remove the inner minimization problem by

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

Maximize the Margin

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

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It's equivalent to solving the minimization problem

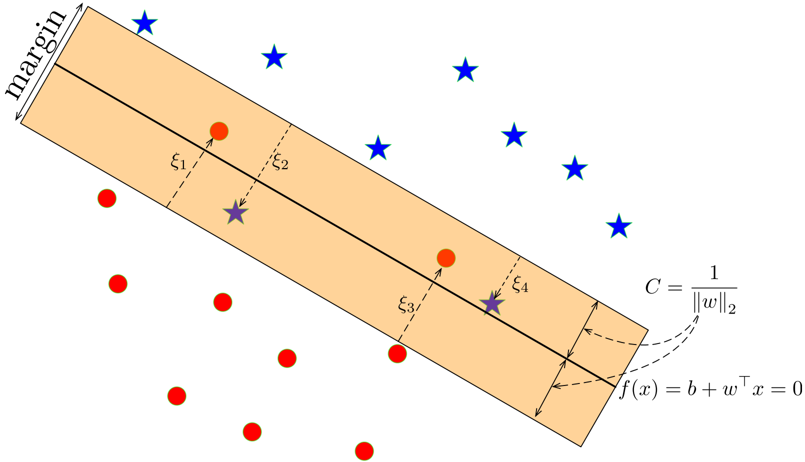
$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|w\|_2^2 \\ \text{subject to} & y_i(w^T x_i + b) \geqslant 1 \quad \text{for all } i \end{array}$$

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:

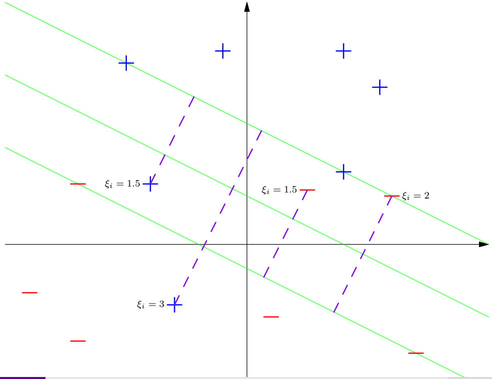
$$
\begin{array}{ll}
\text{minimize} & \frac{1}{2}\|w\|_2^2 + \frac{C}{n}\sum_{i=1}^n \xi_i \\
\text{subject to} & y_i(w^T x_i + b) \geqslant 1 - \xi_i \quad \text{for all } i \\
& \xi_i \geqslant 0 \quad \text{for all } i
\end{array}
$$

- 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:

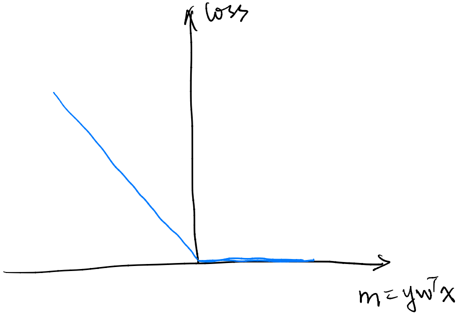
- $\xi_i = 1$: x_i lies on the hyperplane
- $\xi_i = 3$: x_i is past 2 margin width beyond the decision hyperplane



Minimize the Hinge Loss

Perceptron Loss

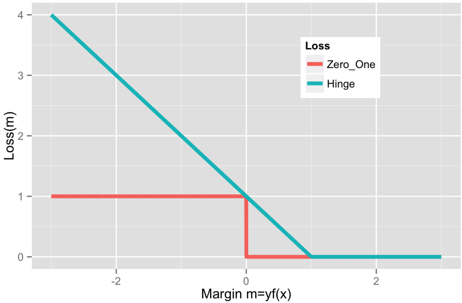
$$\ell(x, y, w) = \max(0, -yw^T x)$$



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 $m < 1$.

SVM as an Optimization Problem

- The SVM optimization problem is equivalent to

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\begin{array}{ll}
\text{minimize} & \frac{1}{2}\|w\|^2 + \frac{c}{n}\sum_{i=1}^{n}\xi_i \\
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Move the constraint into the objective:

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

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- The first term is the L2 regularizer.
- The second term is the Hinge loss.

Using ERM:

- Hypothesis space $\mathcal{F} = \left\{ f(x) = w^T x + b \mid w \in \mathbf{R}^d, b \in \mathbf{R} \right\}$.
- ℓ_2 regularization (Tikhonov style)
- Hinge loss $\ell(m) = \max\{1-m, 0\} = (1-m)_+$
- The SVM prediction function is the solution to

$$\min_{w \in \mathbf{R}^d, b \in \mathbf{R}} \frac{1}{2}||w||^2 + \frac{c}{n}\sum_{i=1}^{n} \max\left(0, 1 - y_i\left[w^T x_i + b\right]\right).$$

- Not differentiable because of the max

Summary

Two ways to derive the SVM optimization problem:

- Maximize the margin
- Minimize the hinge loss with ℓ_2 regularization

Both leads to the minimum norm solution satisfying certain margin constraints.

- **Hard-margin SVM**: all points must be correctly classified with the margin constraints
- **Soft-margin SVM**: allow for margin constraint violation with some penalty