

SVM in Dual Form

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Borrowed most parts from Prof Dale Schuurmans notes and Prof
David Helmbold slides

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Part 1: Background about constrained optimization

Background

Unconstrained optimization of a differentiable function

At the optimal point, the gradient must be zero

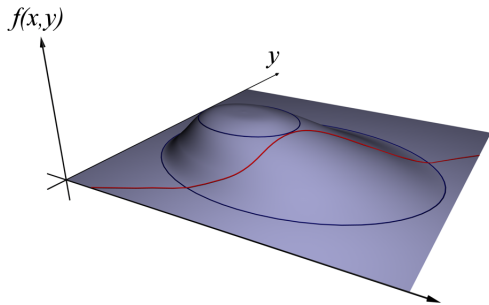
Background

Unconstrained optimization of a differentiable function

At the optimal point, the gradient must be zero

Optimization of a differentiable function with a single equality constraint

At the optimal point, the gradient of function must be parallel to the gradient of constraint.



Background: Constrained optimization

Note: Optional. Supposed to help in understanding the rest.

- When we have an unconstrained problem, we know how to find the local min: Just perform a local descent method.
- How about when we want to solve a **constrained problem**? How do we find the local optimum that satisfy the constraints?
- Example

$$\min_{x_1, x_2} x_1 + x_2 \quad \text{s.t.} \quad x_1^2 + x_2^2 = 2$$

Background: Constrained optimization

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- Find the points in which gradient of objective functions is parallel with the gradient of constraint set.
- Or equivalently (why?) form a function (Lagrangian)

$$\mathcal{L}(x_1, x_2, \lambda) = x_1 + x_2 + \lambda(x_1^2 + x_2^2 - 2)$$

$\nabla \mathcal{L} = \mathbf{0}$, solve for x_1, x_2, λ .

Lagrange Multipliers

Mathematical tool to transform a differentiable constrained optimization problems into optimization problems involving **fewer constraints** but **more variables**.

- How?

- 1 Form a new function, **Lagrangian**, by additively combining the objective function and the constraint.

Example from Last Slide:

$$\mathcal{L}(x_1, x_2, \lambda) = x_1 + x_2 - \lambda(x_1^2 + x_2^2 - 2)$$

- 2 Set the gradient of Lagrangian $\nabla \mathcal{L}$ to zero to find a stationary point of the $\mathcal{L}(x_1, x_2, \lambda)$.
- 3 Solve for x_1, x_2, λ .
- 4 Optimizers of the original problem form a stationary point (i.e. points with zero gradient) of the new problem.

Optimization with equality and inequality constraints

- The case where we have inequality constraints too.
- Form the generalized form of a Lagrangian as below.
- Satisfy **Karush-KuhnTucker(KKT)** conditions!

Primal

$$\min_{\mathbf{w}} \ell(\mathbf{w}) \quad \text{s.t.} \quad A\mathbf{w} \geqslant \mathbf{b}, C\mathbf{w} = \mathbf{d}$$

Lagrangian with multiplier (λ) and multipliers (ν)

$$\mathcal{L}(\mathbf{w}, \lambda, \nu) = \ell(\mathbf{w}) + \lambda^\top (\mathbf{b} - A\mathbf{w}) + \nu^\top (\mathbf{d} - C\mathbf{w})$$

KKT Conditions

1 Stationarity

$$\nabla \mathcal{L}(\mathbf{w}, \lambda, \mathbf{v}) = 0$$

2 Primal feasibility

$$A\mathbf{w} \geq b, C\mathbf{w} = \mathbf{d}$$

3 Dual feasibility

$$\lambda \geq 0$$

4 Complementary slackness

$$\lambda^\top (\mathbf{b} - A\mathbf{w}) = 0$$

That is, for any single inequality constraint either the Lagrange multiplier is zero, or the inequality is tight.

For optimum of the constrained optimization problem, these conditions are satisfied.

Part 2: Deriving the dual for maximum margin classifier.

- Back to machine learning.
- Benefit of deriving dual of SVM
 - Gives another way of solving the optimization problem typically more efficient
 - Gives insight!
 - Again completely convex (Both primal and dual forms of max margin models are completely convex)

Recall: Maximum margin classification, the linearly separable case problem

Given a set of labeled examples, $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_t, y_t)$ where each $\mathbf{x}_i \in \mathbb{R}^n$ and each $y_i \in \{+1, -1\}$, find a weight vector \mathbf{w} and intercept b such that $\text{sign}(\mathbf{w} \bullet \mathbf{x}_i + b) = y_i$ for all i . (assume linearly separable)

Want to maximize the minimum *margin*, but

$$\max_{\mathbf{w}, b} \min_i y_i (\mathbf{w} \bullet \mathbf{x}_i + b)$$

is not well defined (consider doubling \mathbf{w} and b).

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is not well defined (consider doubling \mathbf{w} and b).

functional margin = $y(\mathbf{w} \bullet \mathbf{x} + b)$ depends on scaling

geometric margin = distance between point and hyperplane

$$= \frac{y(\mathbf{w} \bullet \mathbf{x} + b)}{\|\mathbf{w}\|_2}$$

Recall

Want to maximize **geometric margin**: $\min_i \frac{y_i(\mathbf{w} \bullet \mathbf{x}_i + b)}{\|\mathbf{w}\|_2}$

Equivalent to:

$$\min_{\mathbf{w}, b} \|\mathbf{w}\|_2 \quad \text{subject to} \quad y_i(\mathbf{w} \bullet \mathbf{x}_i + b) \geq 1 \text{ for all } i,$$

and to:

$$\min_{\mathbf{w}, b} \frac{1}{2}(\mathbf{w}^\top \mathbf{w}) \quad \text{subject to} \quad \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}) \geq \mathbf{1}$$

Primal Problem

$$\min_{\mathbf{w}, b} \frac{1}{2}(\mathbf{w}^\top \mathbf{w}) \quad \text{subject to} \quad \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}) \geqslant \mathbf{1}$$

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Lagrangian:

$$L(\mathbf{w}, b, \lambda) = \frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}))$$

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Dual problem:

$$\max_{\lambda \succeq \mathbf{0}} \min_{\mathbf{w}, b} \left[\frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1})) \right]$$

Can solve this problem instead of the primal.

$$\max_{\lambda \succeq \mathbf{0}} \min_{\mathbf{w}, b} \underbrace{\frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top \left(\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}) \right)}_{L(\mathbf{w}, b, \lambda)}$$

$$\max_{\lambda \succeq \mathbf{0}} \min_{\mathbf{w}, b} \underbrace{\frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}))}_{L(\mathbf{w}, b, \lambda)}$$

To solve inner min, differentiate $L(\mathbf{w}, b, \lambda)$ with respect to \mathbf{w} and b , and set it to zero:

$$\max_{\lambda \succeq \mathbf{0}} \min_{\mathbf{w}, b} \underbrace{\frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}))}_{L(\mathbf{w}, b, \lambda)}$$

To solve inner min, differentiate $L(\mathbf{w}, b, \lambda)$ with respect to \mathbf{w} and b , and set it to zero:

$$\frac{\partial L(\mathbf{w}, b, \lambda)}{\partial \mathbf{w}} = \mathbf{w} - X^\top \Delta(\mathbf{y})\lambda = 0 \quad \Rightarrow \quad \mathbf{w} = X^\top \Delta(\mathbf{y})\lambda$$

$$\max_{\lambda \succeq \mathbf{0}} \min_{\mathbf{w}, b} \underbrace{\frac{1}{2}(\mathbf{w}^\top \mathbf{w}) + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1}))}_{L(\mathbf{w}, b, \lambda)}$$

To solve inner min, differentiate $L(\mathbf{w}, b, \lambda)$ with respect to \mathbf{w} and b , and set it to zero:

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$$\frac{\partial L(\mathbf{w}, b, \lambda)}{\partial b} = -\lambda^\top \mathbf{y} = 0 \quad \Rightarrow \quad \lambda^\top \mathbf{y} = 0$$

Interesting observations!

- $\mathbf{w} = X^\top \Delta(\mathbf{y})\boldsymbol{\lambda}$ means \mathbf{w} is a weighted sum of examples (like what we had in representer theorem)
- $\boldsymbol{\lambda}^\top \mathbf{y} = 0$ means positive and negative examples have same total weight
- One of Karush-Kuhn-Tucker conditions, **Complementary Slackness**, implies that for each constraint term

$$\lambda_i (1 - y_i(\mathbf{w} \bullet \mathbf{x}_i + b))$$

if $\lambda_i \neq 0$ then the constraint is tight (i.e. $y_i(\mathbf{x}_i^\top \mathbf{w} + b) = 1$), so ...

- $\lambda_i > 0$ only when \mathbf{x}_i is a support vector.
- \mathbf{w} is a weighted sum of (signed) *support vectors*.

Get ready to plug into $L(\mathbf{w}, b, \lambda)$:

Term 1

$$\frac{1}{2} \mathbf{w}^\top \mathbf{w} = \frac{1}{2} \underbrace{\left(X^\top \Delta(\mathbf{y}) \lambda \right)^\top}_{\mathbf{w}^\top} \underbrace{\left(X^\top \Delta(\mathbf{y}) \lambda \right)}_{\mathbf{w}} = \frac{1}{2} \lambda^\top \Delta(\mathbf{y}) X X^\top \Delta(\mathbf{y}) \lambda$$

Term 2

$$\begin{aligned} \lambda^\top \Delta(\mathbf{y}) (X \mathbf{w} + b \mathbf{1}) &= \lambda^\top \Delta(\mathbf{y}) X \underbrace{X^\top \Delta(\mathbf{y}) \lambda}_{\mathbf{w}} + \underbrace{b \lambda^\top \mathbf{y}}_0 \\ &= \lambda^\top \Delta(\mathbf{y}) X X^\top \Delta(\mathbf{y}) \lambda \end{aligned}$$

(Note $\Delta(\mathbf{y}) \mathbf{1} = \mathbf{y}$)

The Dual

$$\max_{\lambda: \lambda \geq 0, \lambda^\top y = 0} \lambda^\top \mathbf{1} - \frac{1}{2} \lambda^\top \Delta(y) X X^\top \Delta(y) \lambda$$

This is a **quadratic programming problem** - can be done numerically.

Recover primal solutions from λ^*

From λ^* , compute $\mathbf{w}^* = X^\top \Delta(y) \lambda^*$, and

From complementary slackness for any $\lambda_i > 0$

Prediction

$$\hat{y} = \text{sign}(x_o^\top \mathbf{w}^* + b) = \text{sign}(x_o^\top X^\top \Delta(y) \lambda + b)$$

Training and prediction kernelized!

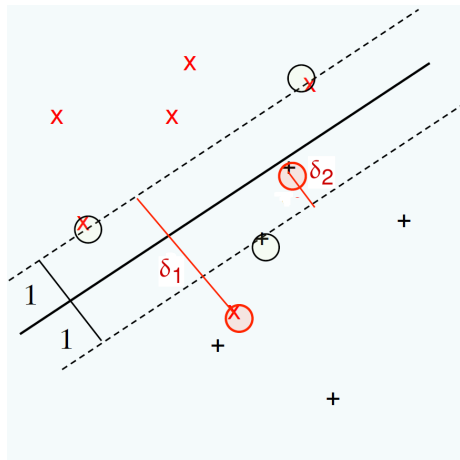
Sparseness

- Only for support vectors are λ_i non-zero – usually few support vectors.
- Removing labeled examples only changes hypothesis if a support vector removed.
- If ℓ out of t examples are support vectors, gives an expected error bound of ℓ/t .

Part 3: Deriving the dual for soft maximum margin classifier.

Recall: Soft margin Idea

- Data doesn't always have good margin
- Allow Margin errors (imperfect classification)
- Let $\delta_i \geq 0$ be error on \mathbf{x}_i
- *Hinge loss* is 0 when margin = 1, increases linearly as margin drops
- trade off accuracy and sum of "errors"



Deriving dual of soft maximum margin classification

Primal

$$\min_{\mathbf{w}, b, \delta} \frac{\beta}{2} \|\mathbf{w}\|_2^2 + \mathbf{1}^\top \delta$$

s.t.

$$\delta \geq \mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + \mathbf{1}b)$$

$$\delta \geq \mathbf{0}$$

Lagrangian with multiplier vectors λ, μ

$$L(\mathbf{w}, b, \delta, \lambda, \mu) = \frac{\beta}{2} \mathbf{w}^\top \mathbf{w} + \mathbf{1}^\top \delta + \lambda^\top (\mathbf{1} - \delta - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1})) - \mu^\top \delta$$

Deriving Dual (Part I: Eliminating δ)

- Write the Lagrangian with all dual and remaining primal variables.

$$L(\mathbf{w}, b, \delta, \lambda, \mu) =$$

$$\frac{\beta}{2} \mathbf{w}^\top \mathbf{w} + \mathbf{1}^\top \delta + \lambda^\top (\mathbf{1} - \delta - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1})) - \mu^\top \delta$$

From KKT Conditions: $\lambda \geq 0, \mu \geq 0$

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- Compute the gradient of Lagrangian wrt variable that you want to eliminate and set it to zero.

$$\frac{dL}{d\delta} = \mathbf{1} - \lambda - \mu = \mathbf{0} \implies \mathbf{1} = \lambda + \mu$$

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- Plug-in and re-write the Lagrangian after eliminating the most recent variable.

$$\implies L(\mathbf{w}, b, \lambda) = \frac{\beta}{2} \mathbf{w}^\top \mathbf{w} + \lambda^\top (\mathbf{1} - \Delta(\mathbf{y})(X\mathbf{w} + b\mathbf{1})), \quad \mathbf{0} \geq \lambda \geq \mathbf{1}$$

Deriving Dual (Part II: eliminating b)

Again a similar procedure

- Write the Lagrangian with all dual and remaining primal variables.

$$L(\mathbf{w}, b, \lambda) = \frac{\beta}{2} \mathbf{w}^\top \mathbf{w} + \lambda^\top ((1 - \Delta(y))(X\mathbf{w} + \mathbf{1}b)), \quad 0 \geq \lambda \geq 1$$

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Deriving dual (Part III: eliminating \mathbf{w})

- Write the Lagrangian with all dual and remaining primal variables.

$$L(\mathbf{w}, \lambda) = \frac{\beta}{2} \mathbf{w}^\top \mathbf{w} + \lambda^\top \left(1 - \Delta(y)(X\mathbf{w}) \right), \quad 0 \leq \lambda \leq 1$$

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- Compute the gradient of Lagrangian wrt variable that you want to eliminate and set it to zero.

$$\frac{dL}{d\mathbf{w}} = \beta \mathbf{w} - X^\top \Delta(\mathbf{y})\lambda = \mathbf{0} \quad \implies \quad \mathbf{w} = \frac{1}{\beta} X^\top \Delta(\mathbf{y})\lambda$$

- Plug-in and write the Lagrangian after eliminating most recent var.

$$\implies \max_{\lambda: 0 \leq \lambda \leq 1, \lambda^\top \mathbf{y} = 0} \lambda^\top \mathbf{1} - \frac{1}{2\beta} \lambda^\top \Delta(\mathbf{y}) X X^\top \Delta(\mathbf{y}) \lambda$$

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Dual

$$\max_{\lambda: 0 \leq \lambda \leq \mathbf{1}, \lambda^\top \mathbf{y} = 0} \lambda^\top \mathbf{1} - \frac{1}{2\beta} \lambda^\top \Delta(\mathbf{y}) X X^\top \Delta(\mathbf{y}) \lambda$$

Recovering primal solutions from dual solutions

Recover \mathbf{w}^*

$$\mathbf{w}^* = \frac{1}{\beta} \mathbf{X}^\top \Delta(\mathbf{y}) \boldsymbol{\lambda}^*$$

Recover b^*

From complementary slackness

For any λ_i s.t. $0 < \lambda_i < 1$ we will have:

- 1 Because $\lambda_i < 1$, and we had from KKT conditions that $\lambda_i + \mu_i = 1 \implies \mu_i > 0 \implies \delta_i = 0$.
- 2 Because $0 < \lambda_i$, $1 - \delta_i - y_i(\mathbf{X}_i \mathbf{w}^* + b^*) = 0$

$$1 = y_i(\mathbf{X}_i \mathbf{w}^* + b^*), \quad y_i \in \{-1, +1\} \implies \frac{1}{y_i} = (\mathbf{X}_i \mathbf{w}^* + b^*)$$

For any $y_i \in \{-1, +1\}$, $y_i^2 = 1$ so $\frac{1}{y_i} = y_i \implies y_i = \mathbf{X}_i \mathbf{w}^* + b^*$

Pick λ_i^* , $0 < \lambda_i^* < 1$ then set $b^* = y_i - \mathbf{X}_i \mathbf{w}^*$

Classification

Given \mathbf{x}_o ,

$$\begin{aligned}\hat{y} &= \text{sign}(\mathbf{x}_o^\top \mathbf{w}^* + b) \\ &= \text{sign}(\mathbf{x}_o^\top X^\top \Delta(\mathbf{y}) + b)\end{aligned}$$

Still kernelized

- Can do all training and testing using λ , XX^\top , $\mathbf{x}^\top X^\top$.
- Don't need \mathbf{w} , nor explicit feature representation X .
- Replace XX^\top with any training kernel K .
- Replace $\mathbf{x}_o X^\top$ with any test kernel K_{test} .

Note: For the soft margin case, we already knew kernelization was possible. Since the maximum soft margin problem is equivalent to L_2 regularized hinge loss. And by representer theorem, L_2 regularized losses could be kernelized.

Where to read?

- Boyd and Vanderberghe (2004), Sec 5.2.3, 5.3.2
- Hastie et al., 2nd ed (2009), Sec. 12.1, 12.2, 12.3.1, 12.3.5
- Bishop (2006), Sec 7.1
- Cherkassky & Mullier (1998), Sec 9.1-9.3