ECE595 / STAT598: Machine Learning I Lecture 20 Support Vector Machine: Duality

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Outline

Support Vector Machine

- Lecture 19 SVM 1: The Concept of Max-Margin
- Lecture 20 SVM 2: Dual SVM
- Lecture 21 SVM 3: Kernel SVM

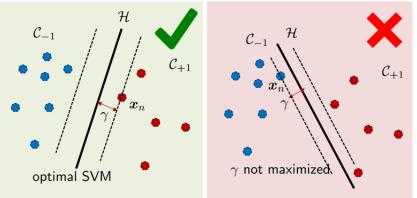
This lecture: Support Vector Machine: Duality

- Lagrange Duality
 - Maximize the dual variable
 - Minimax Problem
 - Toy Example
- Dual SVM
 - Formulation
 - Interpretation

Support Vector Machine

SVM is the solution of this optimization

$$\begin{array}{l} \underset{\boldsymbol{w},w_0}{\text{minimize}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2 \\ \text{subject to } y_j(\boldsymbol{w}^T\boldsymbol{x}_j + w_0) \geq 1, \quad j = 1, \dots, N \end{array}$$



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Lagrange Function

• Goal: Construct the dual problem of

$$\begin{array}{ll} \underset{\boldsymbol{w},w_0}{\text{minimize}} & \frac{1}{2} \|\boldsymbol{w}\|_2^2\\ \text{subject to } & y_j(\boldsymbol{w}^T\boldsymbol{x}_j+w_0) \geq 1, \quad j=1,\ldots,N. \end{array}$$

• Approach: Consider the Lagrangian function

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \underbrace{\frac{1}{2} \|\boldsymbol{w}\|_2^2}_{\text{objective}} + \sum_{j=1}^N \lambda_j \underbrace{\left[1 - y_j(\boldsymbol{w}^T \boldsymbol{x}_j + w_0)\right]}_{\text{constraint}},$$

 \bullet Solution happens at the saddle point of $\mathcal{L}:$

$$abla_{({m w},w_0)}\mathcal{L}({m w},w_0,{m \lambda})={m 0}, \quad \text{and} \quad
abla_{{m \lambda}}\mathcal{L}({m w},w_0,{m \lambda})={m 0}.$$

Lagrangian function

• The Lagrangian function is

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{1}{2} \|\boldsymbol{w}\|_2^2 + \sum_{j=1}^N \lambda_j \underbrace{\left[1 - y_j(\boldsymbol{w}^T \boldsymbol{x}_j + w_0)\right]}_{\leq 0}$$

- Complementarity Condition says
 - $\lambda_j > 0$ and $[1 y_j(w^T x_j + w_0)] = 0$ • $\lambda_j = 0$ and $[1 - y_j(w^T x_j + w_0)] < 0$
- So, if we want ∇_λL(w, w₀, λ) = 0, then must be one of the two cases:

$$\sum_{j=1}^{N} \lambda_j \left[1 - y_j (\boldsymbol{w}^T \boldsymbol{x}_j + w_0) \right] \to \max \quad \text{or} \quad \min$$

- No saddle point because linear in λ .
- But $1 y_j(\boldsymbol{w}^T \boldsymbol{x}_j + w_0) \leq 0$. So unbounded minimum. So must go with maximum.

Primal Problem

• Let λ^* as the maximizer

$$\boldsymbol{\lambda}^* \stackrel{\text{def}}{=} \underset{\boldsymbol{\lambda} \geq \boldsymbol{0}}{\operatorname{argmax}} \left\{ \sum_{j=1}^N \lambda_j \left[1 - y_j (\boldsymbol{w}^T \boldsymbol{x}_j + w_0) \right] \right\}$$

• Then the primal problem is

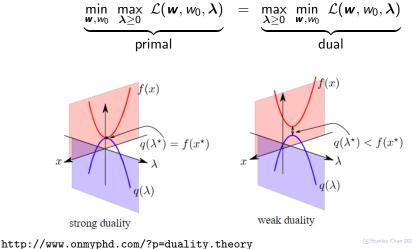
$$\begin{array}{l} \underset{\boldsymbol{w},w_0}{\text{minimize}} \quad \mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda}^*) \\ = \underset{\boldsymbol{w},w_0}{\text{minimize}} \left\{ \frac{1}{2} \|\boldsymbol{w}\|_2^2 + \underset{\boldsymbol{\lambda} \ge \mathbf{0}}{\max} \left\{ \sum_{j=1}^N \lambda_j \left[1 - y_j (\boldsymbol{w}^T \boldsymbol{x}_j + w_0) \right] \right\} \right\} \\ = \underset{\boldsymbol{w},w_0}{\text{minimize}} \left\{ \underset{\boldsymbol{\lambda} \ge \mathbf{0}}{\max} \quad \mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda}) \right\} \end{array}$$

• This is a min-max problem:

$$\min_{\boldsymbol{w},w_0} \max_{\boldsymbol{\lambda} \geq 0} \mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda})$$

Strong Duality

- Recall that our problem is quadratic programming (QP).
- Strong Duality holds for QP:



Toy Example

• The SVM problem

$$\begin{array}{ll} \underset{{\boldsymbol{w}},w_0}{\text{minimize}} & \frac{1}{2} \|{\boldsymbol{w}}\|_2^2\\ \text{subject to} & y_j({\boldsymbol{w}}^T{\boldsymbol{x}}_j+w_0) \geq 1, \quad j=1,\ldots,N. \end{array}$$

in the form of

minimize
$$\|\boldsymbol{u}\|^2$$
, subject to $\boldsymbol{a}_j^T \boldsymbol{u} \ge b_j, \ j = 1, 2, \dots, N$

• Example:

is

$$\underset{u_1,u_2}{\text{minimize}} \quad u_1^2 + u_2^2, \quad \text{subject to} \quad \begin{bmatrix} 1 & 2 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \ge \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

• Can we write down its dual problem?

Toy Example

• Lagrangian function is

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{\lambda}) \stackrel{\text{def}}{=} u_1^2 + u_2^2 + \lambda_1(2 - u_1 - 2u_2) - \lambda_2 u_1 - \lambda_3 u_3$$

• Minimize over **u**:

$$\frac{\partial \mathcal{L}}{\partial u_1} = 0 \quad \Rightarrow \quad u_1 = \frac{\lambda_1 + \lambda_2}{2}$$
$$\frac{\partial \mathcal{L}}{\partial u_2} = 0 \quad \Rightarrow \quad u_2 = \frac{2\lambda_1 + \lambda_3}{2}.$$

• Plugging into the Lagrangian function yields

$$\begin{array}{ll} \underset{\boldsymbol{\lambda}}{\text{maximize}} & \mathcal{L}(\boldsymbol{\lambda}) = -\frac{5}{4}\lambda_1^2 - \frac{1}{4}\lambda_2^2 - \frac{1}{4}\lambda_3^2 - \frac{1}{2}\lambda_1\lambda_2 - \lambda_1\lambda_3 + 2\lambda_1\\ \text{subject to} & \boldsymbol{\lambda} \geq 0. \end{array}$$

• Primal is QP. Dual is also QP.

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Have We Gained Anything?

• Here is the dual problem:

$$\begin{array}{ll} \underset{\lambda}{\text{maximize}} & \mathcal{L}(\lambda) = -\frac{5}{4}\lambda_1^2 - \frac{1}{4}\lambda_2^2 - \frac{1}{4}\lambda_3^2 - \frac{1}{2}\lambda_1\lambda_2 - \lambda_1\lambda_3 + 2\lambda_1 \\ \text{subject to} & \lambda \geq 0. \end{array}$$

These terms are all negative! So we must have λ₂ = λ₃ = 0.
This gives

$$\begin{array}{ll} \underset{\lambda_1\geq 0}{\text{maximize}} & -\frac{5}{4}\lambda_1^2+2\lambda_1. \end{array}$$

which is maximized at $\lambda_1 = \frac{4}{5}$.

• Plugging into the primal yields

$$u_1 = \frac{\lambda_1 + \lambda_2}{2} = \frac{2}{5}$$
, and $u_2 = \frac{2\lambda_1 + \lambda_3}{2} = \frac{4}{5}$.

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Dual of SVM

• We want to find the dual problem of

$$\begin{array}{ll} \underset{\boldsymbol{w},w_0}{\text{minimize}} & \frac{1}{2} \|\boldsymbol{w}\|_2^2 \\ \text{subject to } y_j(\boldsymbol{w}^T\boldsymbol{x}_j+w_0) \geq 1, \quad j=1,\ldots,N. \end{array}$$

• We start with the Lagrangian function

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\lambda}) \stackrel{\text{def}}{=} rac{1}{2} \|\boldsymbol{w}\|_2^2 + \sum_{j=1}^N \lambda_j \left[1 - y_j (\boldsymbol{w}^T \boldsymbol{x}_j + w_0)
ight].$$

• Let us **minimize** over (**w**, w₀):

$$abla_{\boldsymbol{w}}\mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda}) = \boldsymbol{w} - \sum_{j=1}^N \lambda_j y_j \boldsymbol{x}_j = \boldsymbol{0}$$

 $abla_{w_0}\mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda}) = \sum_{j=1}^N \lambda_j y_j = 0.$

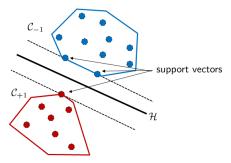
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Interpreting
$$\nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\lambda}) = 0$$

• The first result suggests that

$$\boldsymbol{w} = \sum_{j=1}^N \lambda_j y_j \boldsymbol{x}_j.$$

• This is support vector: λ_j is either $\lambda_j = 0$ or $\lambda_j > 0$.



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Interpreting $\nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\lambda}) = 0$

• The complementarity condition states that

$$\lambda_j^* \left[1 - y_j (\boldsymbol{w^*}^T \boldsymbol{x}_j + \boldsymbol{w}_0^*) \right] = 0, \quad \text{for} \quad j = 1, \dots, N.$$

• If
$$1 - y_j(\boldsymbol{w}^{*T}\boldsymbol{x}_j + w_0^*) > 0$$
, then $\lambda_j^* = 0$

- If $\lambda_j^* > 0$, then $1 y_j(\boldsymbol{w}^{*T}\boldsymbol{x}_j + w_0^*) = 0$
- So you can define the support vector set:

$$\mathcal{V} \stackrel{\mathsf{def}}{=} \{ j \mid \lambda_j^* > \mathsf{0} \}.$$

So the optimal weight is

$$\boldsymbol{w}^* = \sum_{j \in \mathcal{V}} \lambda_j^* y_j \boldsymbol{x}_j.$$

The Lagrangian function is

$$\mathcal{L}(\boldsymbol{w}^*, \boldsymbol{w}_0^*, \boldsymbol{\lambda}) = \frac{1}{2} \|\boldsymbol{w}^*\|_2^2 + \sum_{j=1}^N \lambda_j \left[1 - y_j ((\boldsymbol{w}^*)^T \boldsymbol{x}_j + \boldsymbol{w}_0) \right]$$
$$= \frac{1}{2} \left\| \sum_{j=1}^N \lambda_j y_j \boldsymbol{x}_j \right\|_2^2$$
$$+ \sum_{j=1}^N \lambda_j \left[1 - y_j \left(\left(\sum_{i=1}^n \lambda_i y_i \boldsymbol{x}_i \right)^T \boldsymbol{x}_j + \boldsymbol{w}_0 \right) \right]$$

• We can show that

$$A = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$
$$B = \sum_{j=1}^{N} \lambda_j - \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j - \underbrace{\left(\sum_{j=1}^{N} \lambda_j y_j\right)}_{=0} w_0$$

• and we can show that

$$A + B = \sum_{j=1}^{N} \lambda_j + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j y_i y_j \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j$$

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• Therefore, the dual problem is

$$\begin{array}{ll} \underset{\lambda \geq 0}{\text{maximize}} & -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_{i} \lambda_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j} + \sum_{j=1}^{N} \lambda_{j} \\ \\ \text{subject to} & \sum_{j=1}^{N} \lambda_{j} y_{j} = 0. \end{array}$$

• If you prefer matrix-vector:

$$\begin{array}{ll} \underset{\lambda \geq 0}{\text{maximize}} & -\frac{1}{2} \lambda^T \boldsymbol{Q} \lambda + \boldsymbol{1}^T \lambda \\ \\ \text{subject to } \boldsymbol{y}^T \boldsymbol{\lambda} = \boldsymbol{0}. \end{array}$$

• We can combine the constraints ${m \lambda} \geq 0$ and ${m y}^{{\sf T}} {m \lambda} = {m 0}$ as

$$A\lambda \geq 0.$$

• $\mathbf{y}^T \boldsymbol{\lambda} = 0$ means

$$\mathbf{y}^{\mathsf{T}} \mathbf{\lambda} \geq 0$$
, and $\mathbf{y}^{\mathsf{T}} \mathbf{\lambda} \leq 0$.

• Thus, we can write $\boldsymbol{y}^{T}\boldsymbol{\lambda}=0$ as

$$\begin{bmatrix} \boldsymbol{y}^{\mathsf{T}} \\ -\boldsymbol{y}^{\mathsf{T}} \end{bmatrix} \boldsymbol{\lambda} \geq \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{0} \end{bmatrix}.$$

• Therefore, the matrices ${oldsymbol Q}$ and ${oldsymbol A}$ are

$$\boldsymbol{Q} = \begin{bmatrix} y_1 y_1 \boldsymbol{x}_1^T \boldsymbol{x}_1 & \dots & y_1 y_N \boldsymbol{x}_1^T \boldsymbol{x}_N \\ y_2 y_1 \boldsymbol{x}_2^T \boldsymbol{x}_1 & \dots & y_2 y_N \boldsymbol{x}_2^T \boldsymbol{x}_N \\ \vdots & \vdots & \vdots \\ y_N y_1 \boldsymbol{x}_N^T \boldsymbol{x}_1 & \dots & y_N y_N \boldsymbol{x}_N^T \boldsymbol{x}_N \end{bmatrix} \text{ and } \boldsymbol{A} = \begin{bmatrix} \boldsymbol{y}^T \\ -\boldsymbol{y}^T \\ \boldsymbol{I} \end{bmatrix}$$

So How to Solve the SVM Problem?

• You look at the dual problem

$$\begin{array}{ll} \underset{\boldsymbol{\lambda}}{\text{maximize}} & -\frac{1}{2}\boldsymbol{\lambda}^{\mathsf{T}}\boldsymbol{Q}\boldsymbol{\lambda} + \boldsymbol{1}^{\mathsf{T}}\boldsymbol{\lambda}\\ \text{subject to} & \boldsymbol{A}\boldsymbol{\lambda} \geq \boldsymbol{0}. \end{array}$$

- You get the solution λ^* .
- Then compute **w***:

$$\boldsymbol{w}^* = \sum_{j \in \mathcal{V}} \lambda_j^* y_j \boldsymbol{x}_j.$$

• \mathcal{V} is the set of support vectors: $\lambda_j > 0$.

Are We Done Yet?

- Not quite.
- We still need to find out w_0^* .
- Pick any support vector $x^+ \in C_+$ and $x^- \in C_-$.
- Then we have

$$w^T x^+ + w_0 = +1$$
, and $w^T x^- + w_0 = -1$.

• Sum them, we have $\boldsymbol{w}^{T}(\boldsymbol{x}^{+}+\boldsymbol{x}^{-})+2w_{0}=0$, which means

$$w_0^* = -\frac{(x^+ + x^-)^T w^*}{2}$$

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Summary of Dual SVM

Primal $\underset{\boldsymbol{w},w_0}{\text{minimize}} \quad \frac{1}{2} \|\boldsymbol{w}\|_2^2$ subject to $y_i(\mathbf{w}^T \mathbf{x}_i + w_0) > 1$, i = 1, ..., N. Strong Duality $\min_{\boldsymbol{w},w_0} \max_{\boldsymbol{\lambda} \geq 0} \mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda} \geq 0} \min_{\boldsymbol{w},w_0} \mathcal{L}(\boldsymbol{w},w_0,\boldsymbol{\lambda})$ primal dual Dual $\begin{array}{ll} \underset{\boldsymbol{\lambda} \geq 0}{\text{maximize}} & -\frac{1}{2} \sum_{i=1}^{N} \sum_{i=1}^{N} \lambda_{i} \lambda_{j} y_{i} y_{j} \boldsymbol{x}_{i}^{T} \boldsymbol{x}_{j} + \sum_{j=1}^{N} \lambda_{j} \end{array}$ subject to $\sum_{j=1}^{N} \lambda_j y_j = 0.$

21/31

Summary of Dual SVM

• The weights are computed as

$$\boldsymbol{w}^* = \sum_{j=1}^N \lambda_j^* y_j \boldsymbol{x}_j.$$

- This is support vector: λ_j is either $\lambda_j = 0$ or $\lambda_j > 0$.
- Pick any support vector $x^+ \in C_+$ and $x^- \in C_-$.
- Then we have

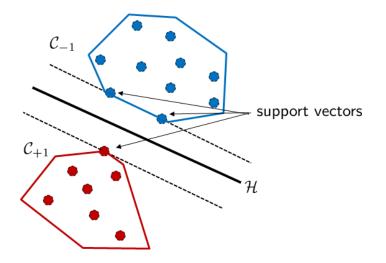
$$w^T x^+ + w_0 = +1$$
, and $w^T x^- + w_0 = -1$.

• Sum them, we have $\boldsymbol{w}^T(\boldsymbol{x}^+ + \boldsymbol{x}^-) + 2w_0 = 0$, which means

$$w_0^* = -\frac{(x^+ + x^-)^T w^*}{2}$$

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Summary of Dual SVM



Reading List

Support Vector Machine

- Mustafa, Learning from Data, e-Chapter
- Duda-Hart-Stork, Pattern Classification, Chapter 5.5
- Chris Bishop, Pattern Recognition, Chapter 7.1
- UCSD Statistical Learning

http://www.svcl.ucsd.edu/courses/ece271B-F09/

Appendix

Inequality Constrained Optimization

Inequality constrained optimization:

$$\begin{array}{ll} \underset{\boldsymbol{x} \in \mathbb{R}^n}{\text{minimize}} & f(\boldsymbol{x}) \\ \text{subject to} & g_i(\boldsymbol{x}) \ge 0, \qquad i = 1, \dots, m \\ & h_j(\boldsymbol{x}) = 0, \qquad j = 1, \dots, k. \end{array}$$

Requires a function: Lagrangian function

$$\mathcal{L}(\mathbf{x},\boldsymbol{\mu},\boldsymbol{\nu}) \stackrel{\text{def}}{=} f(\mathbf{x}) - \sum_{i=1}^{m} \mu_i g_i(\mathbf{x}) - \sum_{j=1}^{k} \nu_j h_j(\mathbf{x}).$$

 $\mu \in \mathbb{R}^m$ and $\nu \in \mathbb{R}^k$ are called the Lagrange multipliers or the dual variables.

Karush-Kahn-Tucker Conditions

If (x^*, μ^*, ν^*) is the solution to the constrained optimization, then all the following conditions should hold:

- (i) $\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \mu^*, \nu^*) = \mathbf{0}.$
 - Stationarity.
 - The primal variables should be stationary.
- (ii) $g_i(\mathbf{x}^*) \ge 0$ and $h_j(\mathbf{x}^*) = 0$ for all i and j.
 - Primal Feasibility.
 - Ensures that constraints are satisfied.
- (iii) $\mu_i^* \ge 0$ for all *i* and *j*.
 - Dual Feasibility.
 - Require $\mu_i^* \ge 0$; but no constraint on ν_i^* .

(iv) $\mu_i^* g_i(\mathbf{x}^*) = 0$ for all *i* and *j*.

- Complementary Slackness
- Either $\mu_i^* = 0$ or $g_i(\mathbf{x}^*) = 0$ (or both).

KKT Condition is a first order **necessary** condition.

Example: ℓ_2 -minimization with two constraints

Solve the following least squares over positive quadrant problem.

$$\begin{array}{l} \underset{\boldsymbol{x} \in \mathbb{R}^n}{\text{minimize}} \quad \frac{1}{2} \| \boldsymbol{x} - \boldsymbol{b} \|^2, \\ \text{subject to } \boldsymbol{x}^T \mathbf{1} = 1, \quad \text{and} \quad \boldsymbol{x} \ge \mathbf{0}. \end{array}$$

$$(1)$$

```
%MATLAB code: Use CVX to solve min ||x-b|| s.t. sum(x) = 1, x >= 0.
cvx_begin
  variable x(n)
  minimize( norm(x-b, 2) )
  subject to
     sum(x) == 1;
     x >= 0;
cvx_end
```

Analytic Solution

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \gamma) = \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|^2 - \boldsymbol{\lambda}^T \mathbf{x} - \gamma (1 - \mathbf{x}^T \mathbf{1}).$$

Stationarity suggests that:

$$abla_{\mathbf{x}}\mathcal{L}(\mathbf{x},\boldsymbol{\lambda},\gamma) = \mathbf{x} - \mathbf{b} - \boldsymbol{\lambda} + \gamma \mathbf{1} = \mathbf{0}$$

This means

$$\boldsymbol{x} = \boldsymbol{b} + \boldsymbol{\lambda} - \gamma \boldsymbol{1}$$
 or $x_i = b_i + \lambda_i - \gamma$.

The **complementary slackness** implies $\lambda_i x_i = 0$.

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These three cases can be re-written as:

- If $b_i > \gamma$, then $x_i = b_i \gamma$;
- If $b_i = \gamma$, then $x_i = 0$;
- If $b_i < \gamma$, then $x_i = 0$.

Compactly written as

$$\mathbf{x} = \max(\mathbf{b} - \gamma \mathbf{1}, \mathbf{0}).$$

Primal feasibility implies that

$$\mathbf{x}^T \mathbf{1} = 1, \qquad \Leftrightarrow \qquad \sum_{i=1}^n x_i = 1.$$

Therefore, γ needs to satisfy the equation

$$\sum_{i=1}^n \max(b_i - \gamma, 0) = 1,$$

which can be found by doing a root-finding of

$$g(\gamma) = \sum_{i=1}^{n} \max(b_i - \gamma, 0) - 1.$$

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Non-CVX Implementation

```
%MATLAB code: solve min ||x-b|| s.t. sum(x) = 1, x >= 0.
n = 10;
b = randn(n,1);
fun = @(gamma) myfun(gamma,b);
gamma = fzero(fun,0);
x = max(b-gamma,0);
```

where the function myfun is defined as

function y = myfun(gamma,b)
y = sum(max(b-gamma,0))-1;