Function Approximation Methods-V

CS771: Introduction to Machine Learning

Purushottam Kar

Outline of today's discussion

PART I

- Revisit Lagrangian duality
- Apply duality to SVMs
- Observe a beautiful connection b/w CD and SGD
- See how some state-of-the-art solvers for SVMs are built

PART II

- Learn how to model data (data features that is)
- Look at the naïve Bayes technique for supervised problems
- Get introduced to the GMM technique for unsupervised problems

Duality

How to take the problem you want to solve
... and convert it to a problem you can solve

Fenchel, Lagrange, Wolfe, Pontryagin

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Duality

How to take the problem you want to solve
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The Lagrangian

The Lagrangian

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w})$$

$$\text{s.t. } g(\mathbf{w}) \leq 0$$

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$$\hat{\mathbf{w}} = \arg\min \sum_{i=1}^{n} \left(y^i - \langle \mathbf{w}, \mathbf{x}^i \rangle\right)^2$$

$$s.t. \ \|\mathbf{w}\|_2 \leq r$$

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Want $g(\mathbf{w}) \geq 0$?
$-g(\mathbf{w}) \leq 0$

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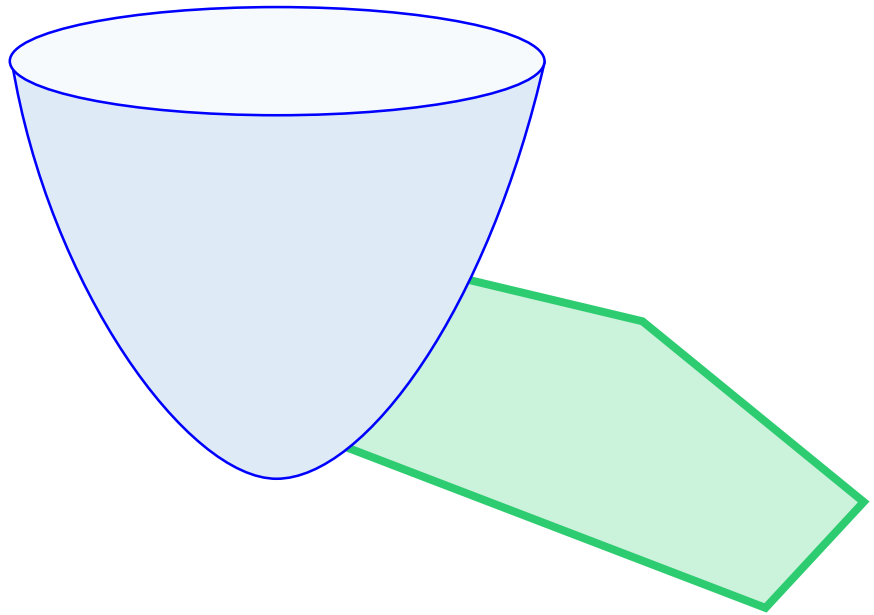
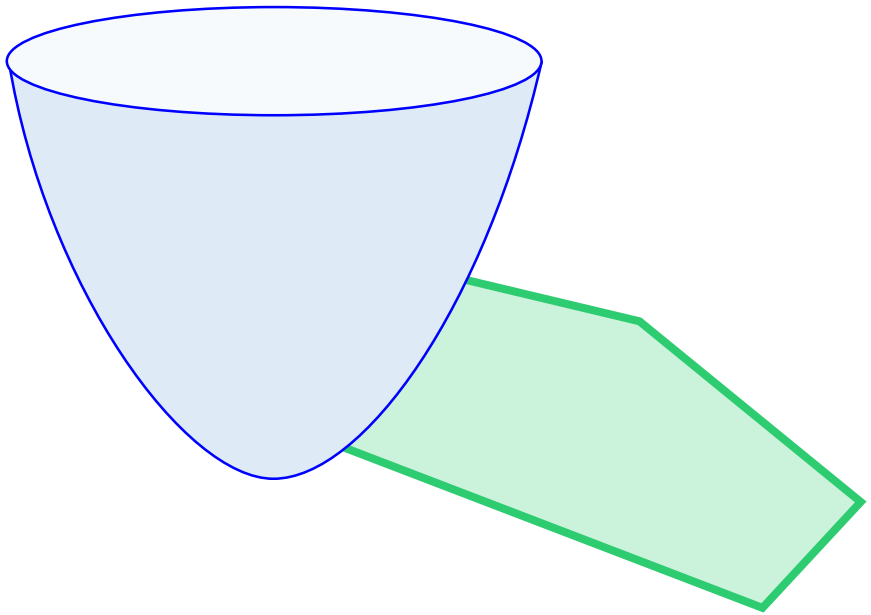


The Lagrangian

$$\hat{\mathbf{w}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\arg\min} \; f(\mathbf{w}) + r(\mathbf{w})$$



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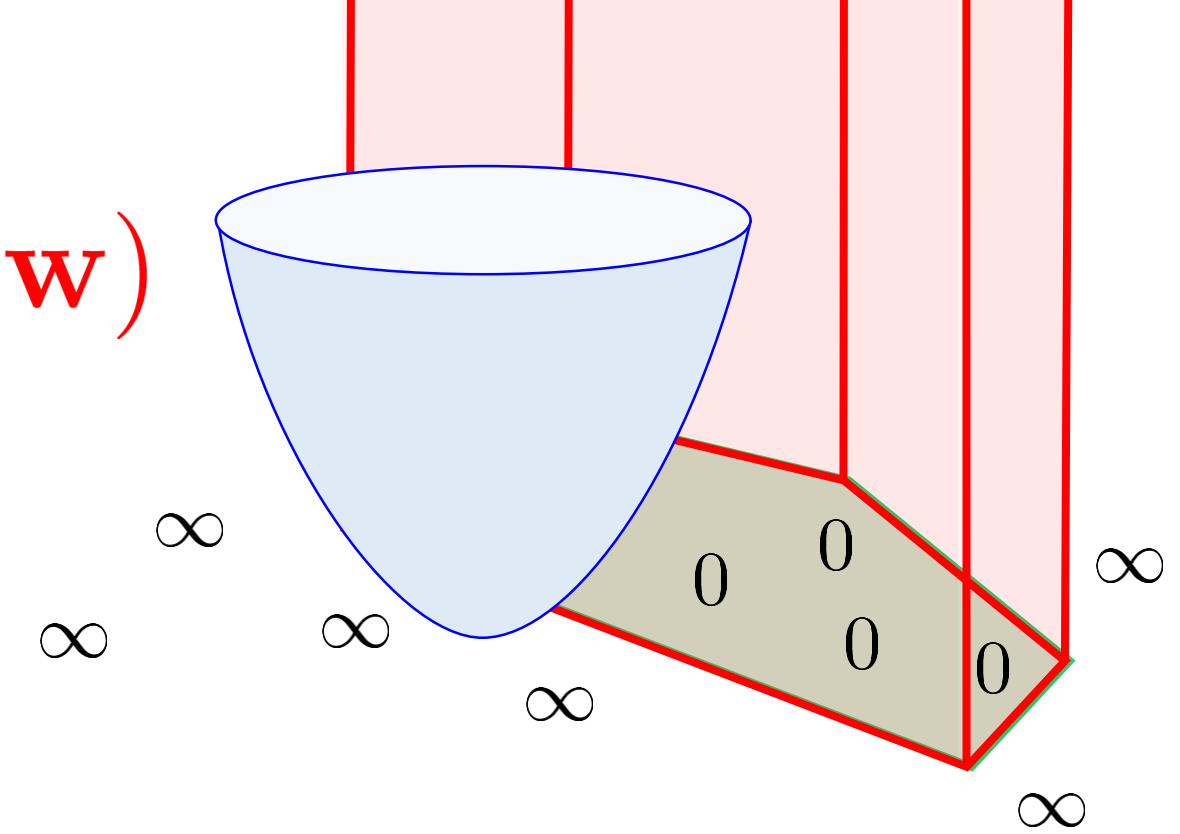
Barrier Function



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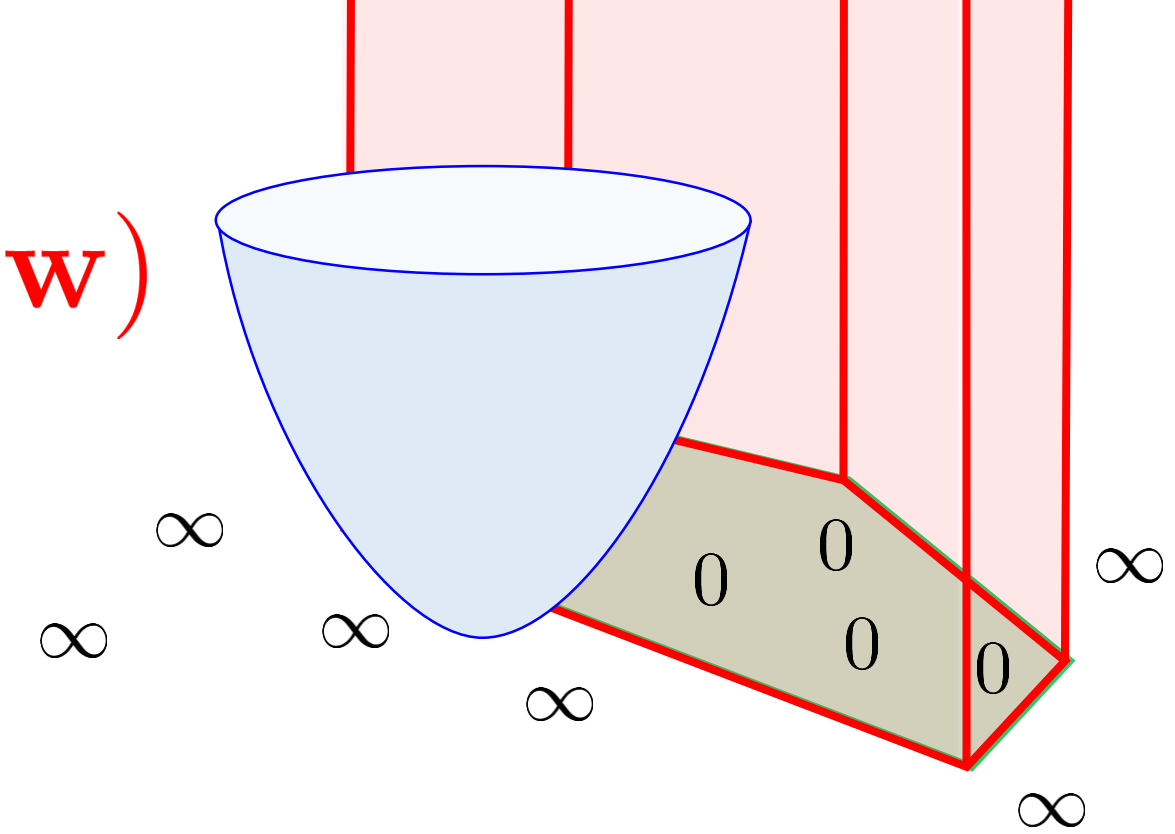

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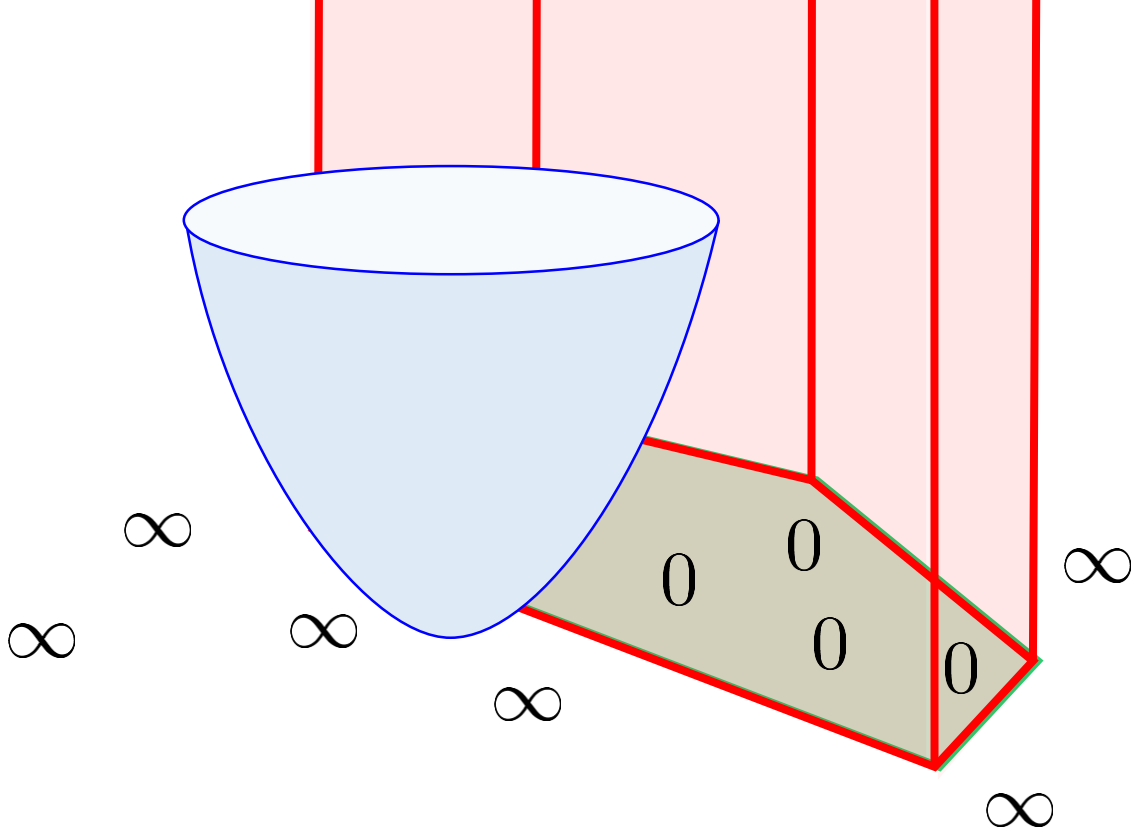

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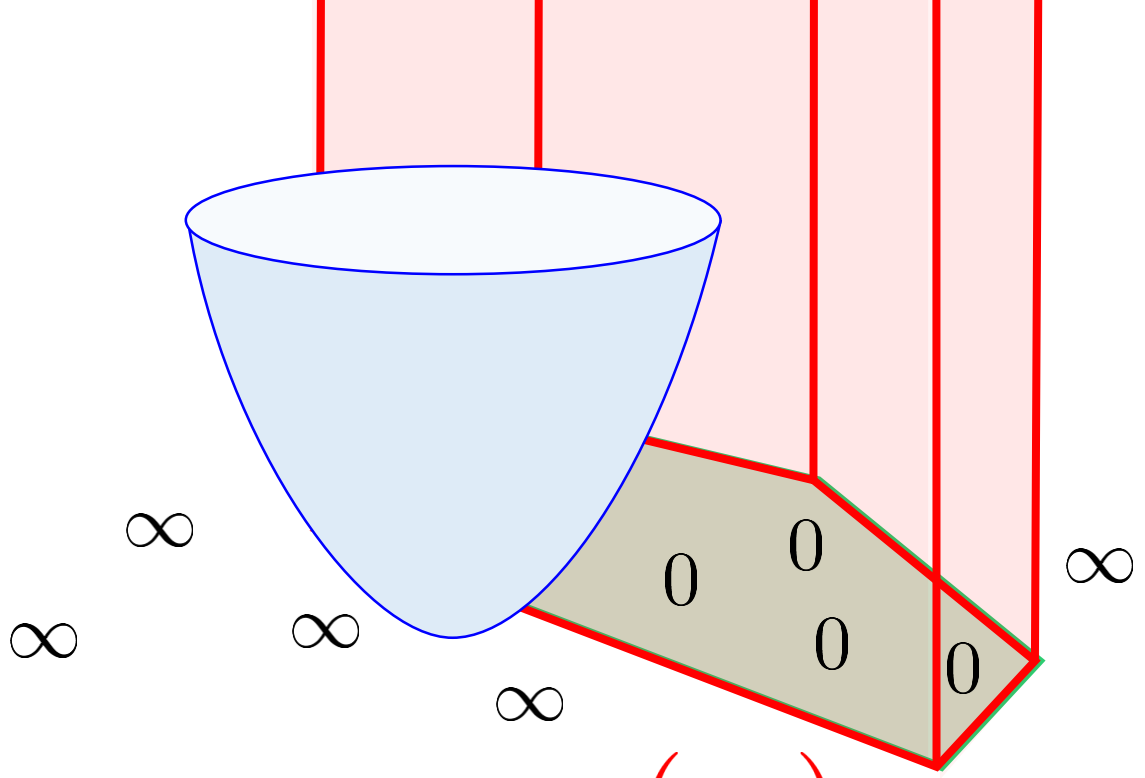

$$\arg\max_{\alpha \geq 0} \alpha \cdot g(\mathbf{w})$$

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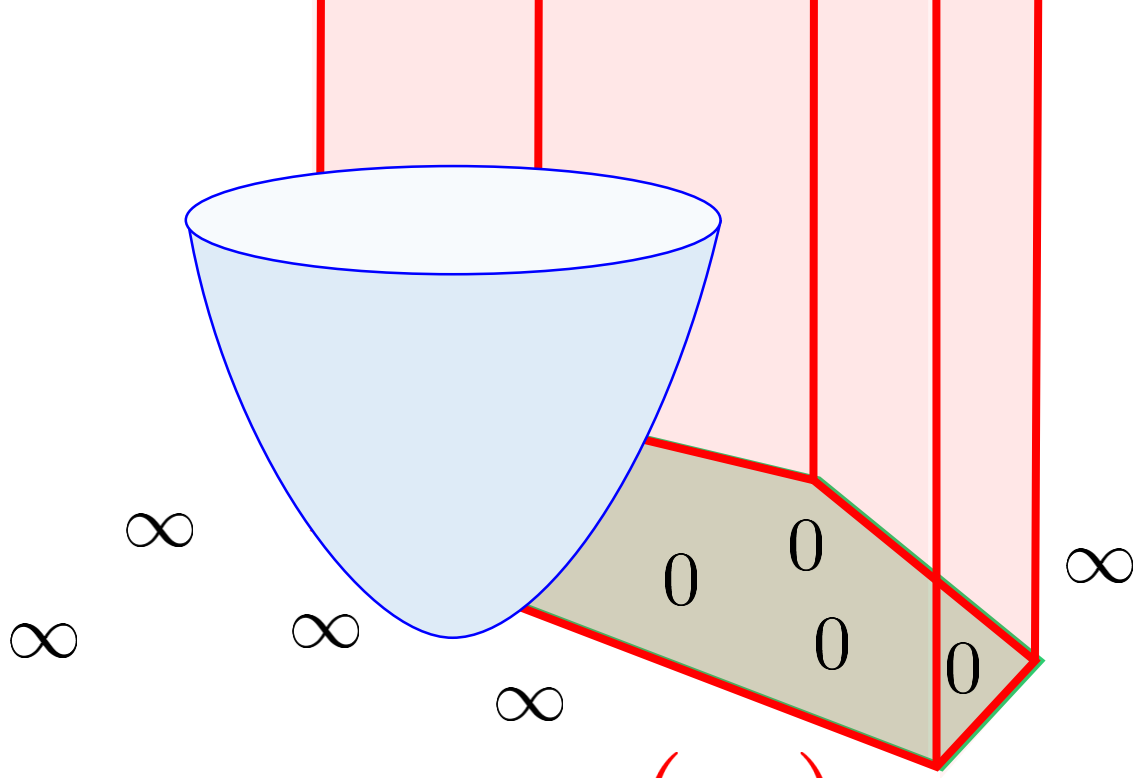

$$\arg\max_{\alpha \geq 0} \alpha \cdot g(\mathbf{w})$$

∞ if $g(\mathbf{w}) > 0$

The Lagrangian

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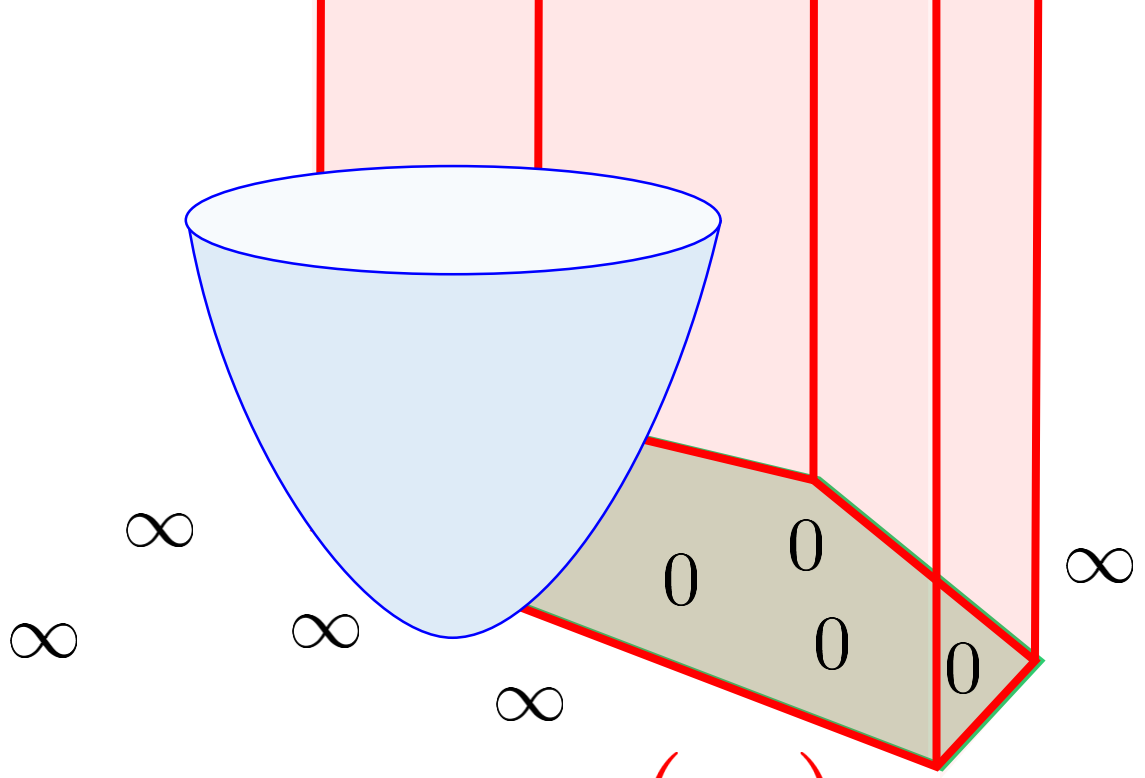
$$\text{s.t. } g(\mathbf{w}) \leq 0$$



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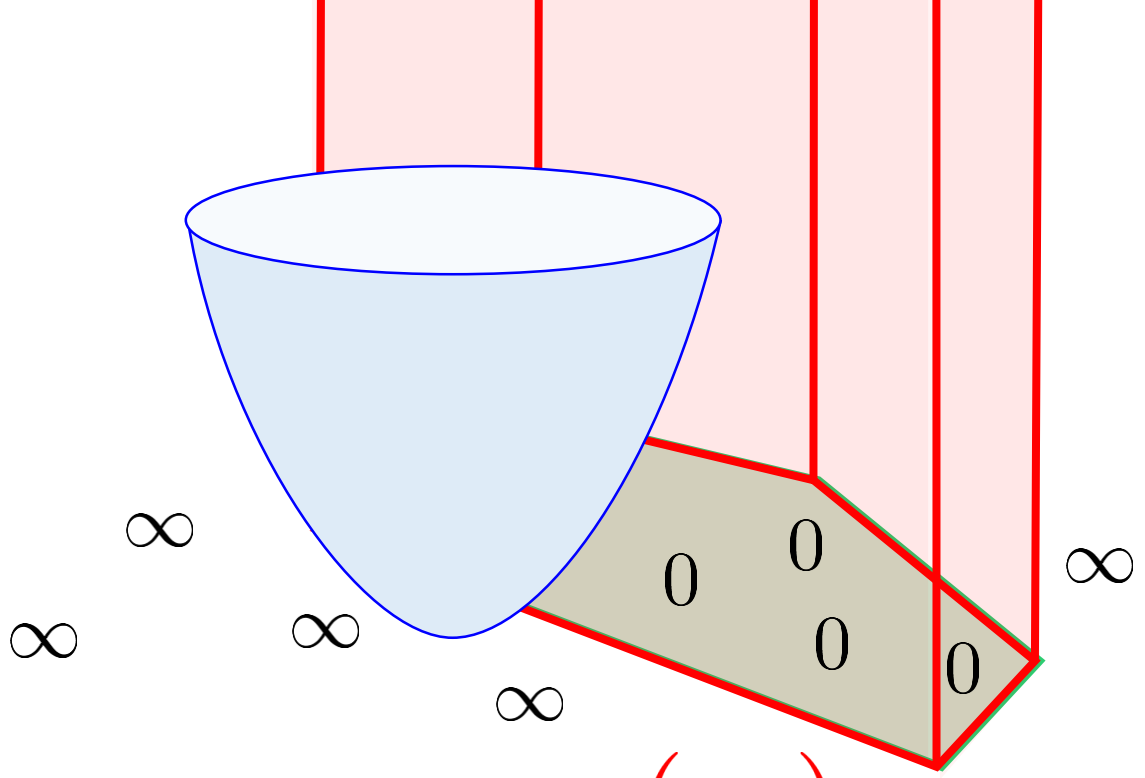


$$f(\mathbf{w}) + \arg\max_{\alpha\geq 0} \alpha \cdot g(\mathbf{w})$$

∞ if $g(\mathbf{w}) > 0$

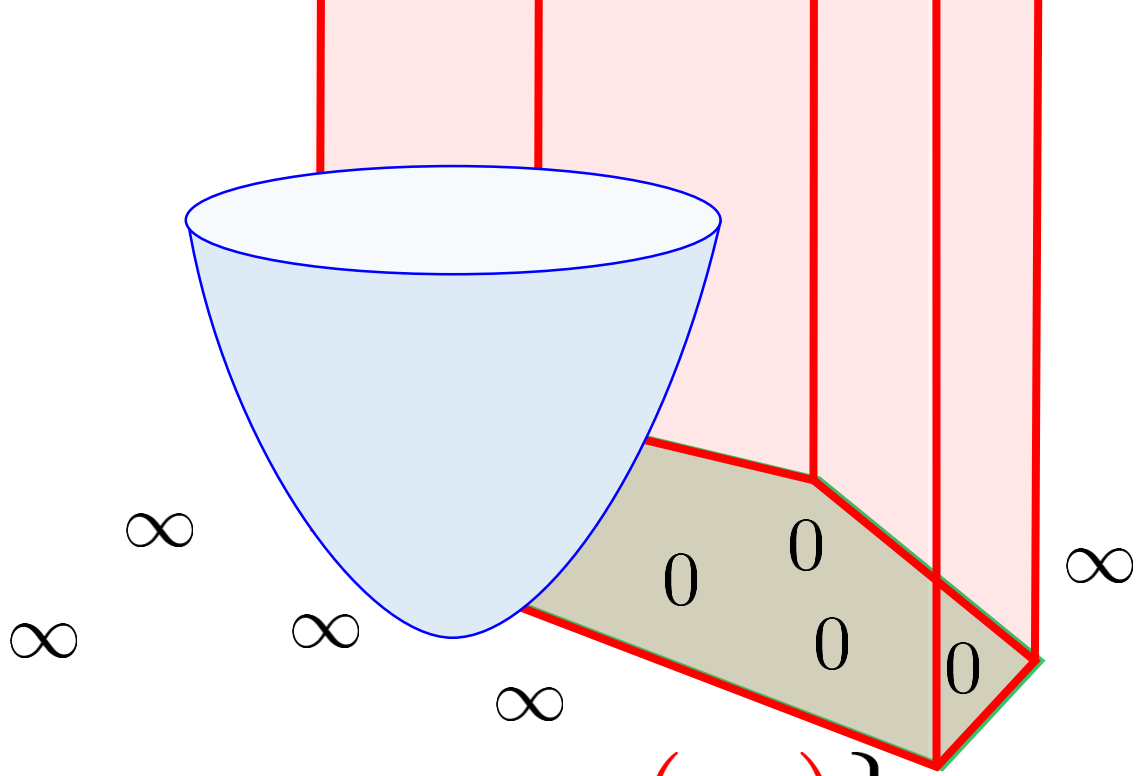
0 if $g(\mathbf{w}) \leq 0$

The Lagrangian

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}\in\mathbb{R}^d} f(\mathbf{w})$$

$$\text{s.t. } g(\mathbf{w}) \leq 0$$

$$\arg\min_{\mathbf{w}\in\mathbb{R}^d} \{f(\mathbf{w}) + \arg\max_{\alpha\geq 0} \alpha \cdot g(\mathbf{w})\}$$



$\alpha \geq 0$

∞ if $g(\mathbf{w}) > 0$

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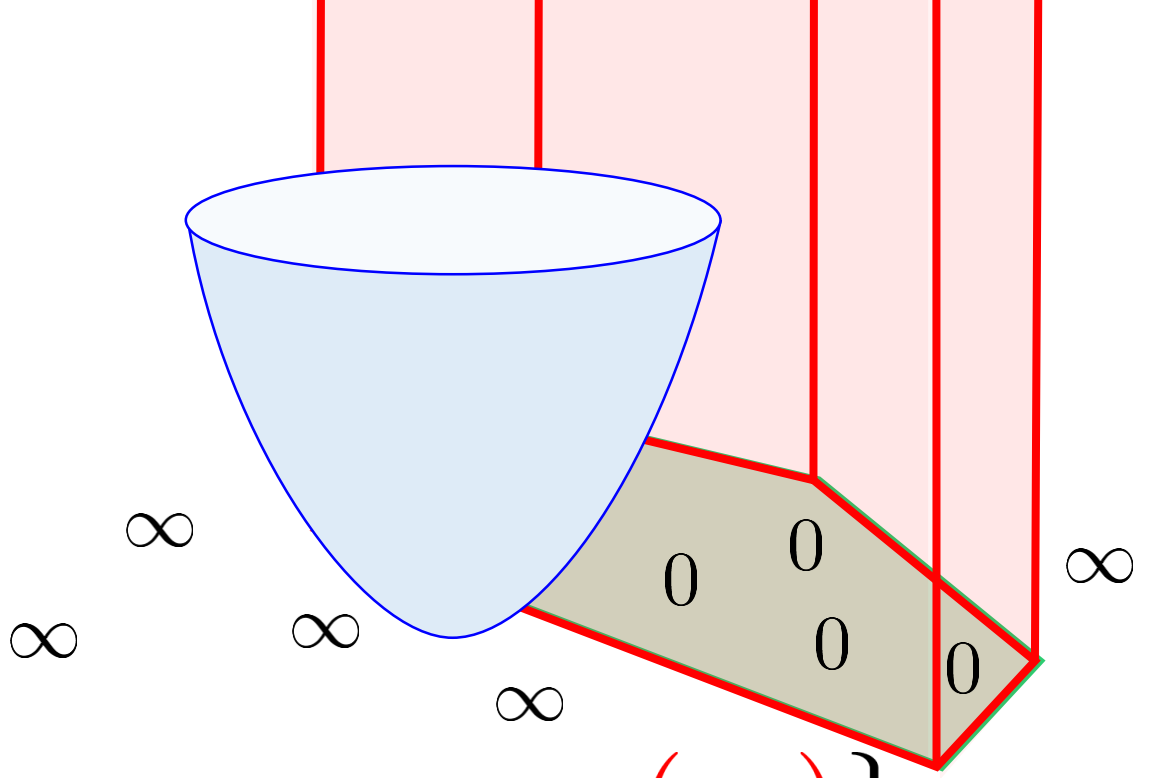

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \{ f(\mathbf{w}) + \arg\max_{\alpha \geq 0} \alpha \cdot g(\mathbf{w}) \}$$

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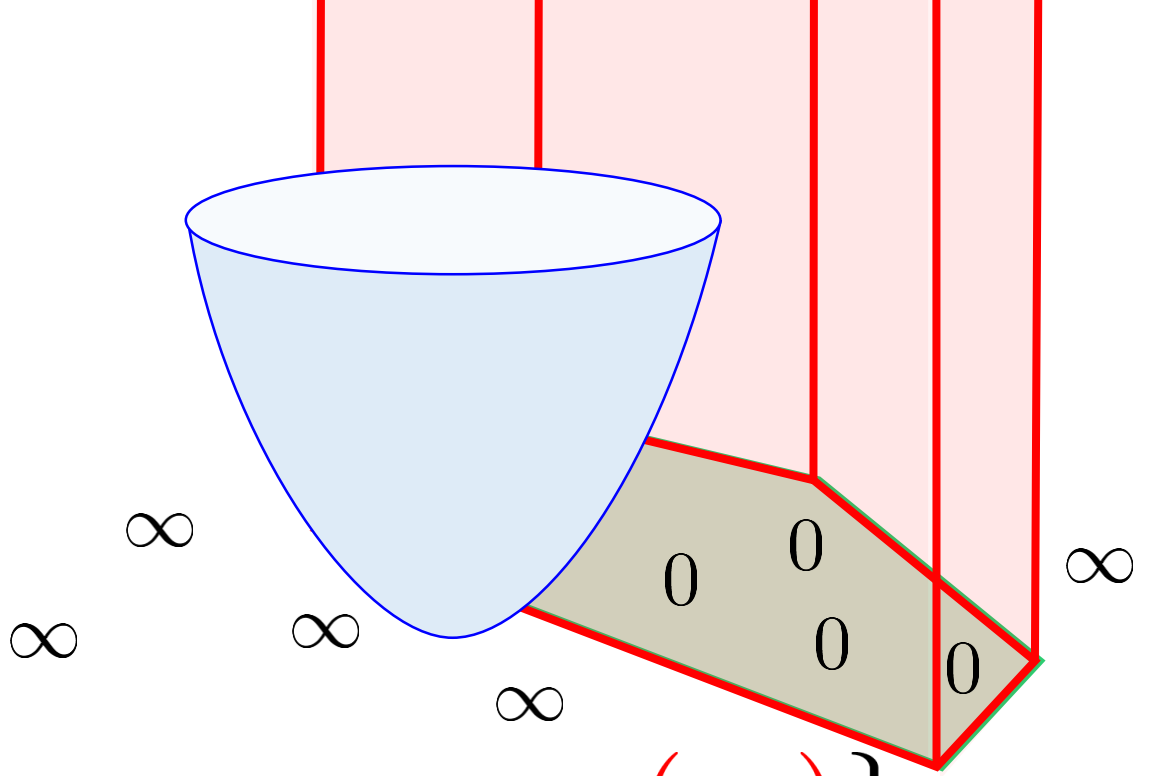

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Exercise

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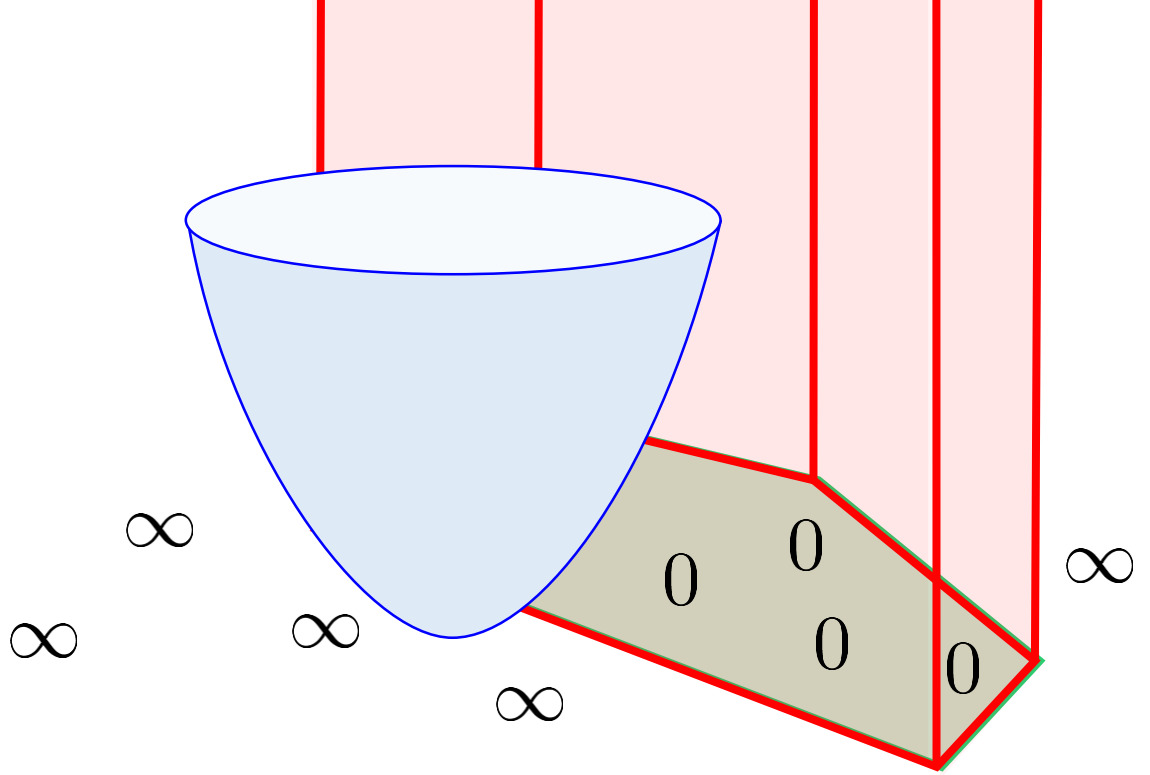

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \left\{ \arg\max_{\alpha \geq 0} \left\{ f(\mathbf{w}) + \alpha \cdot g(\mathbf{w}) \right\} \right\}^{\infty}$$

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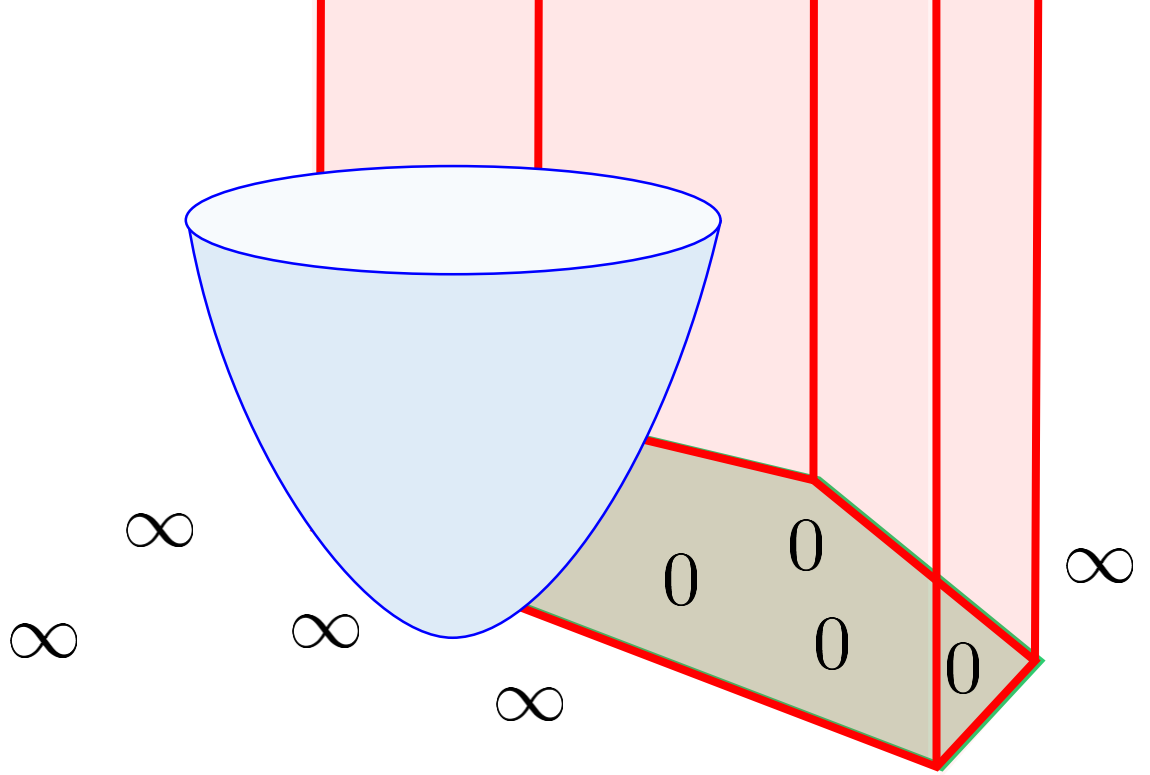

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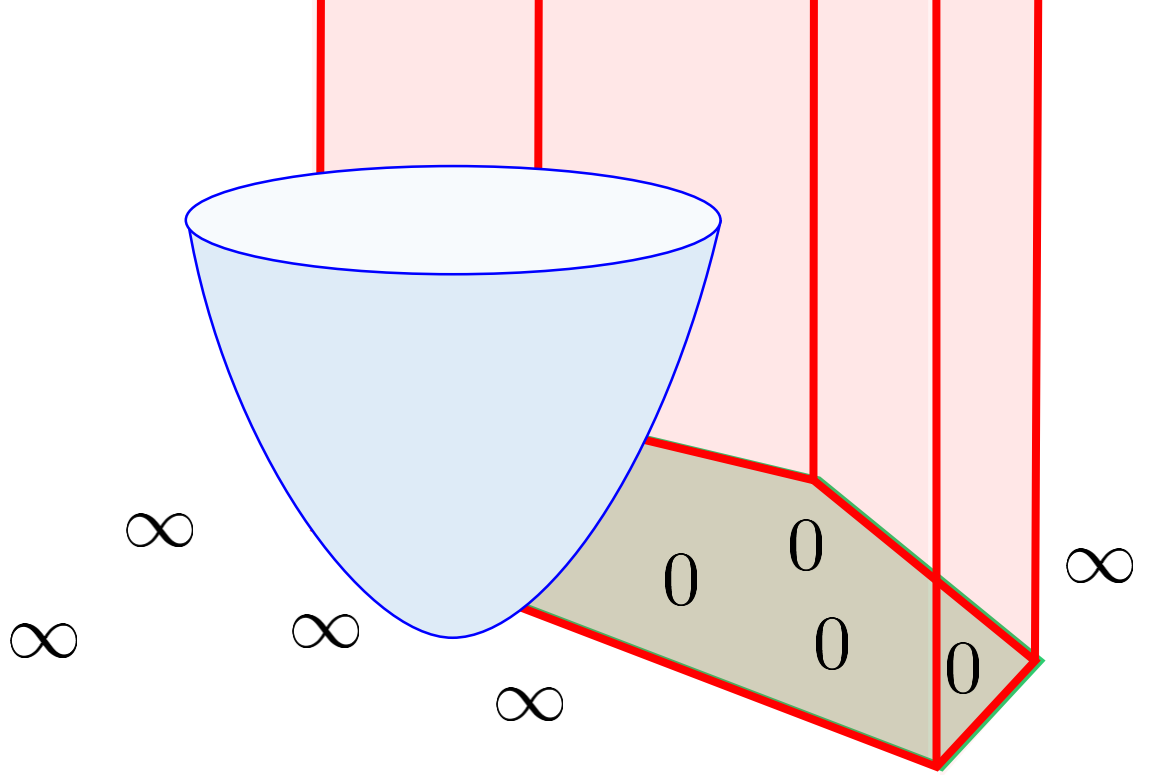

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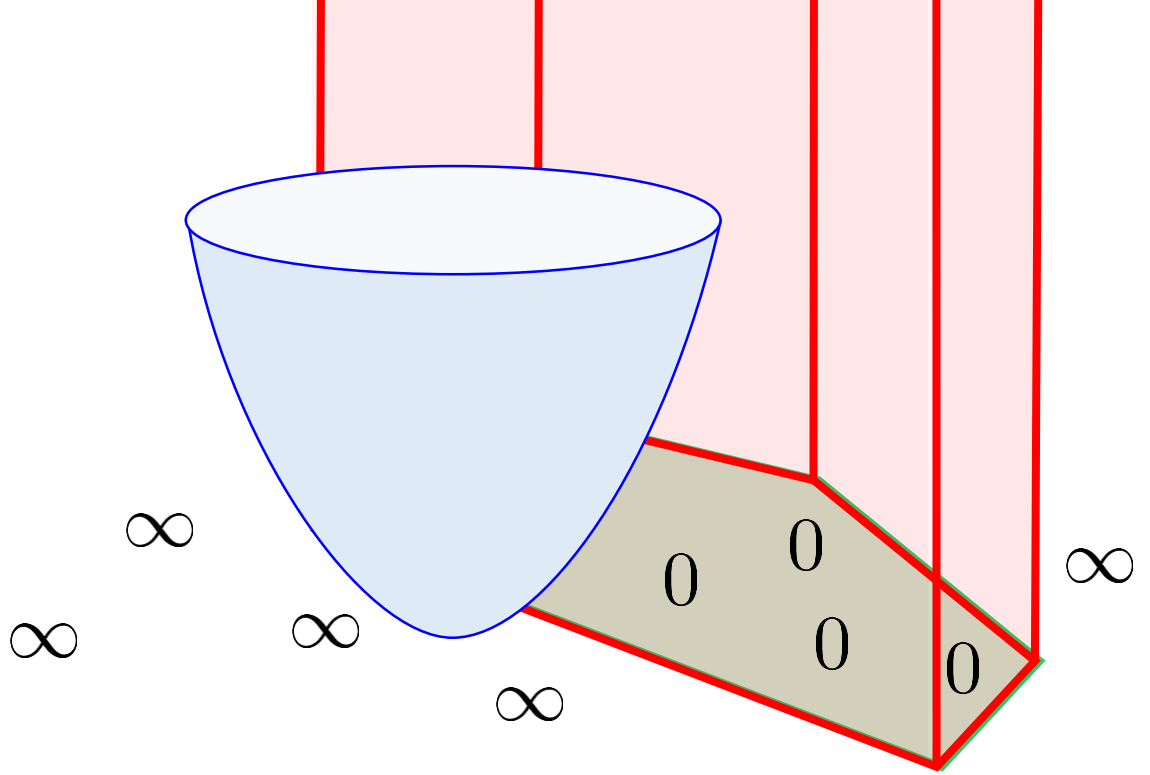

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Lagrange multiplier

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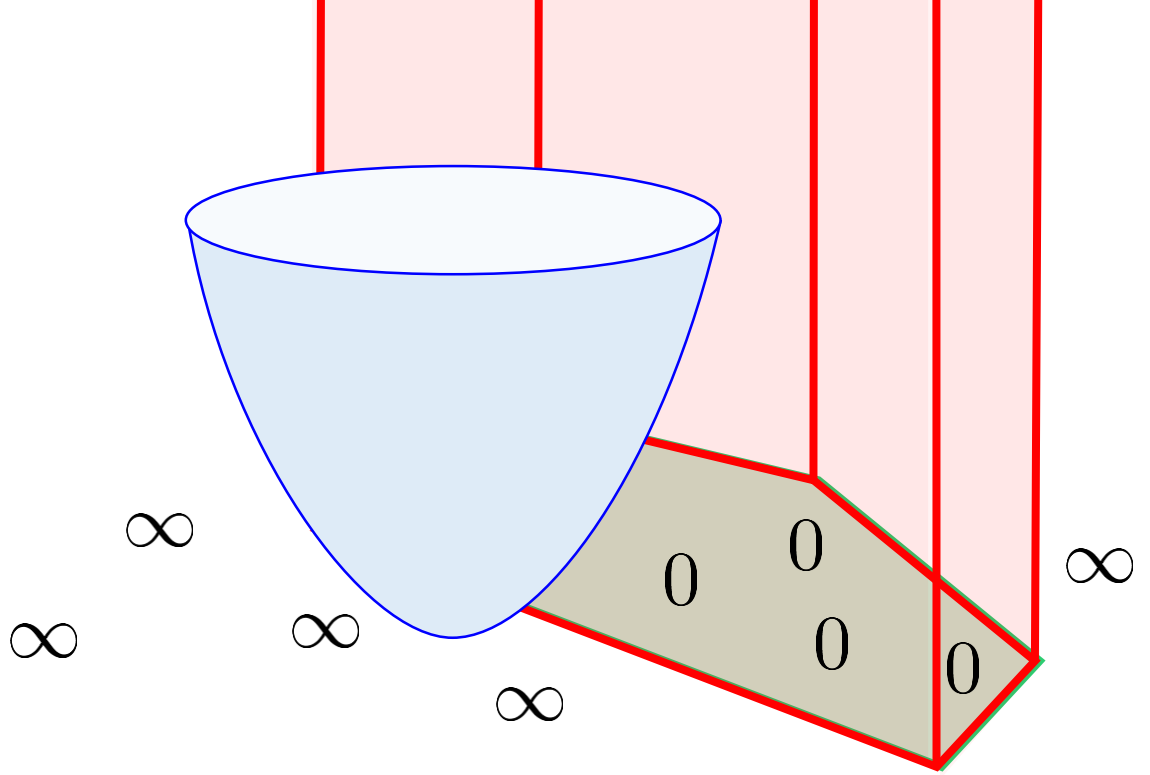

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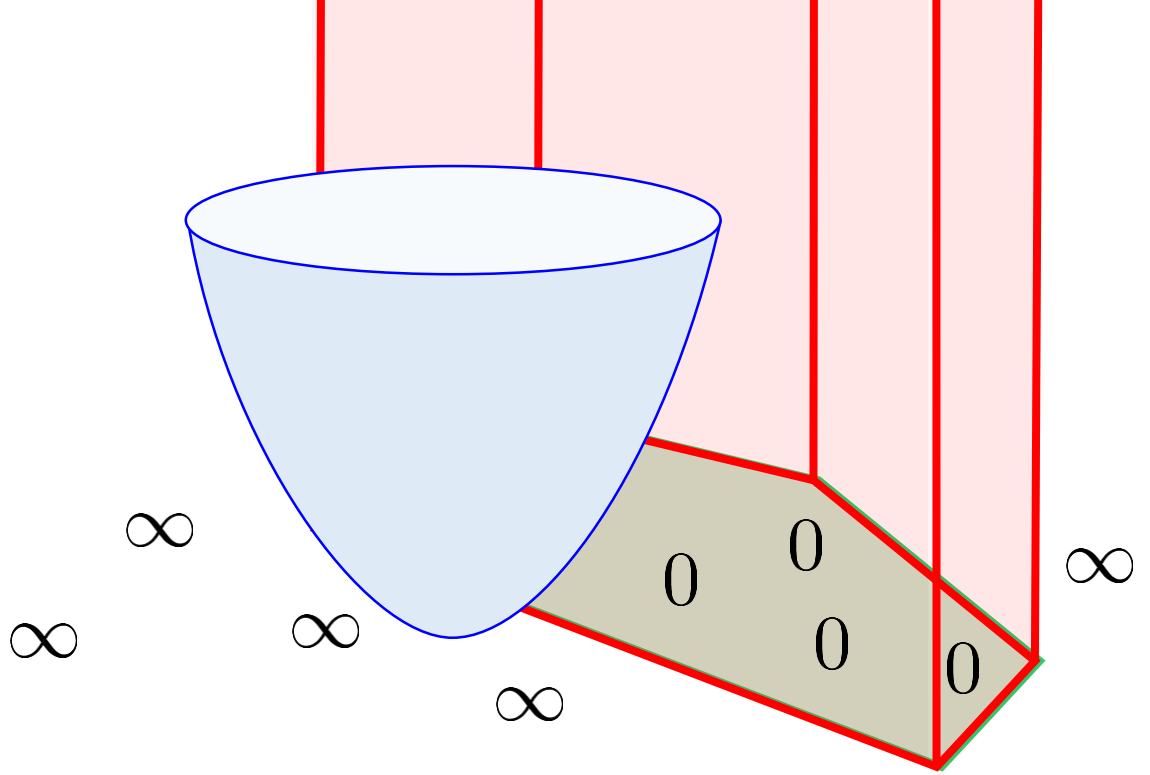

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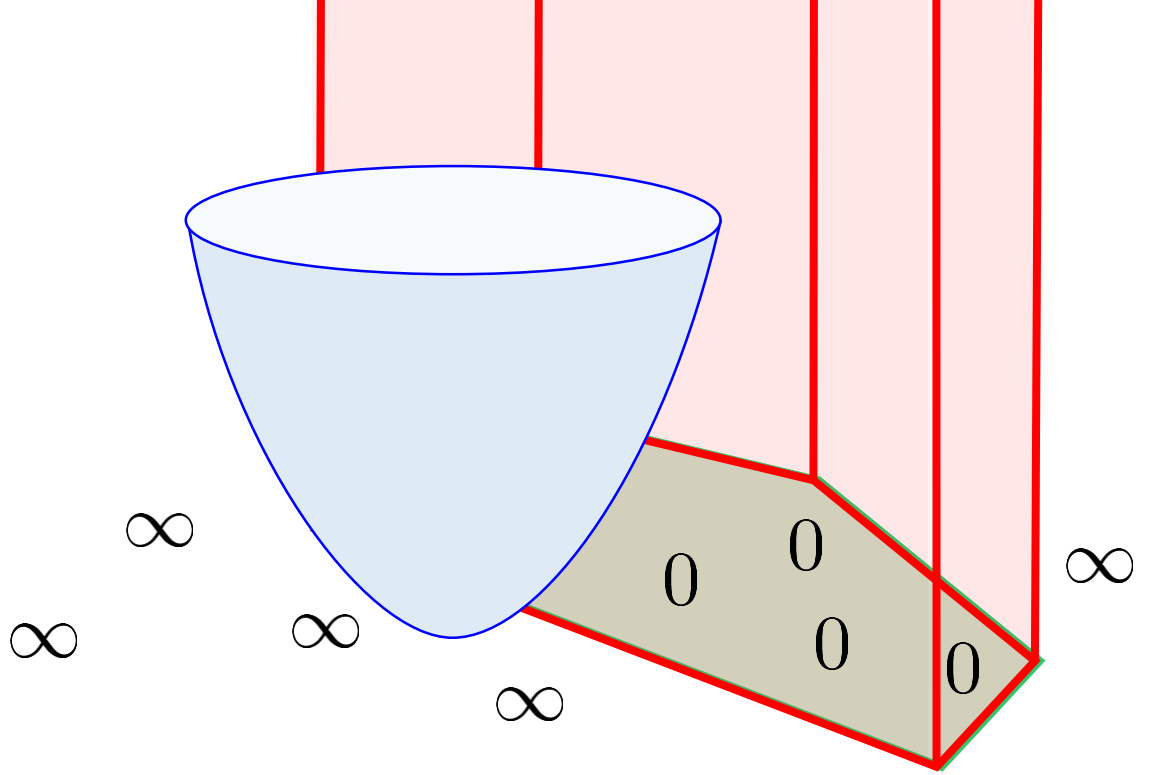

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Lagrange multiplier

Primal problem

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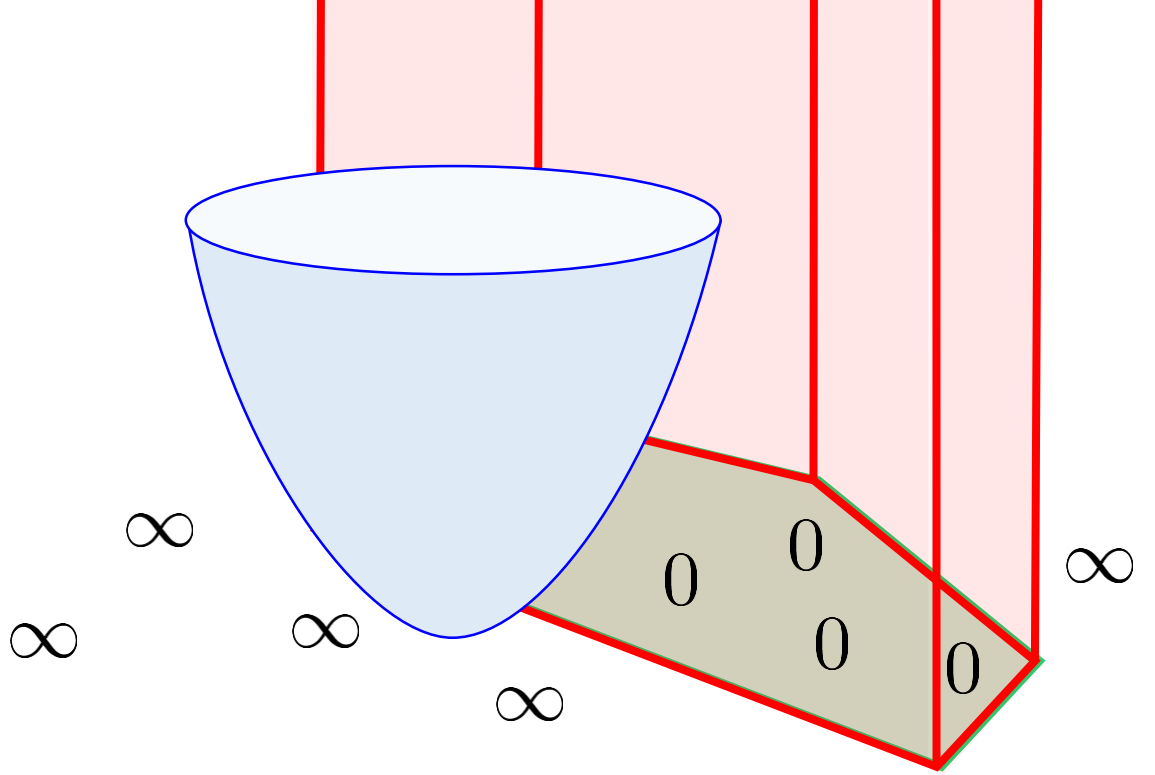

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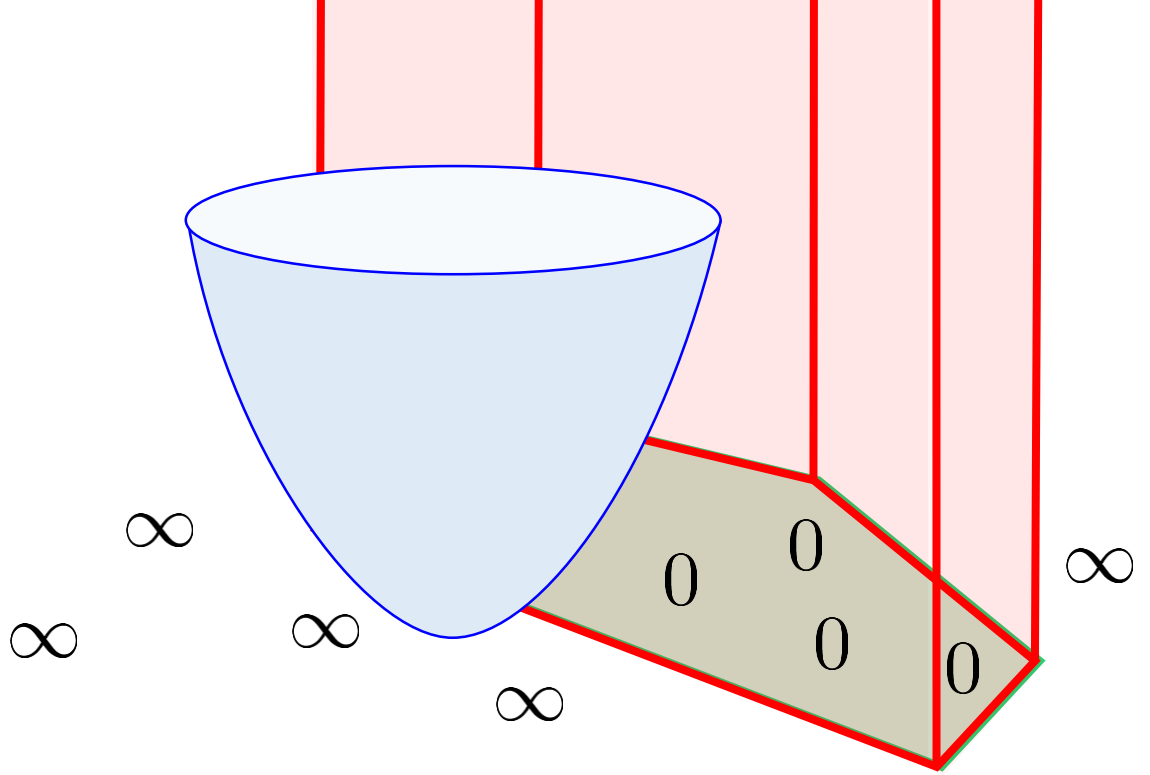

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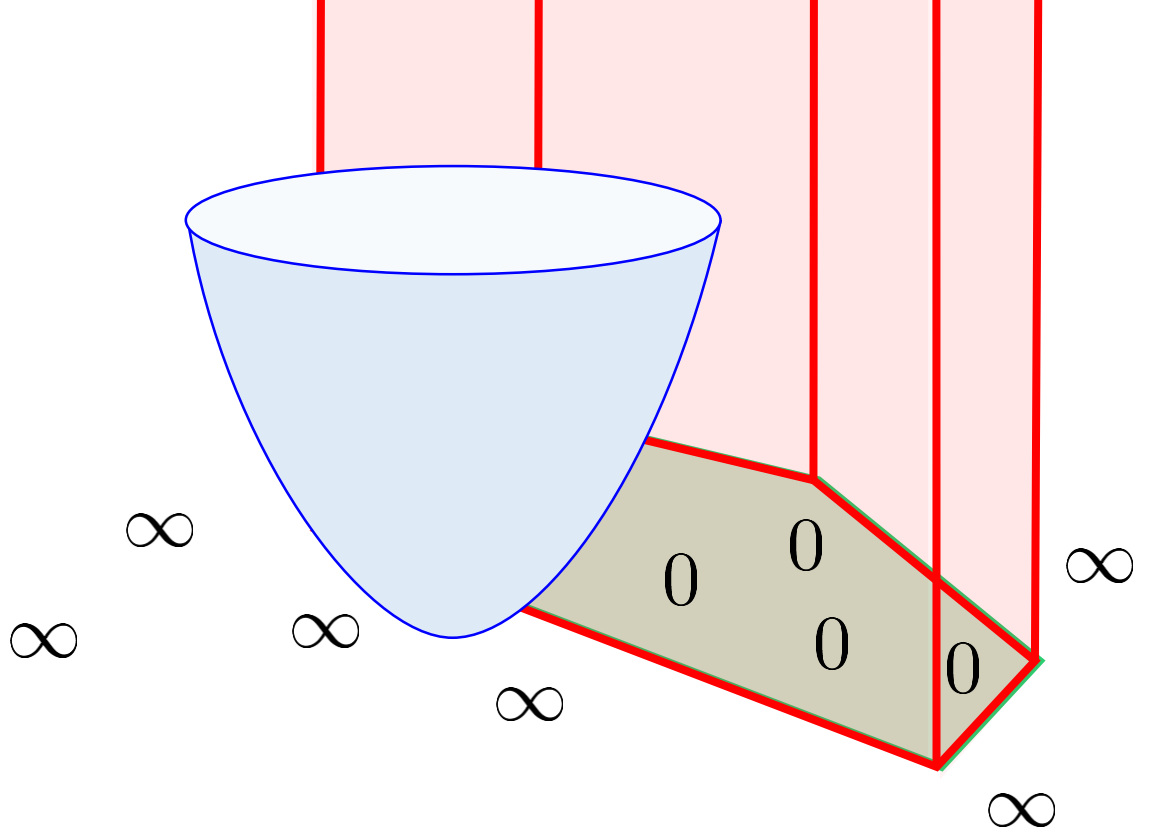

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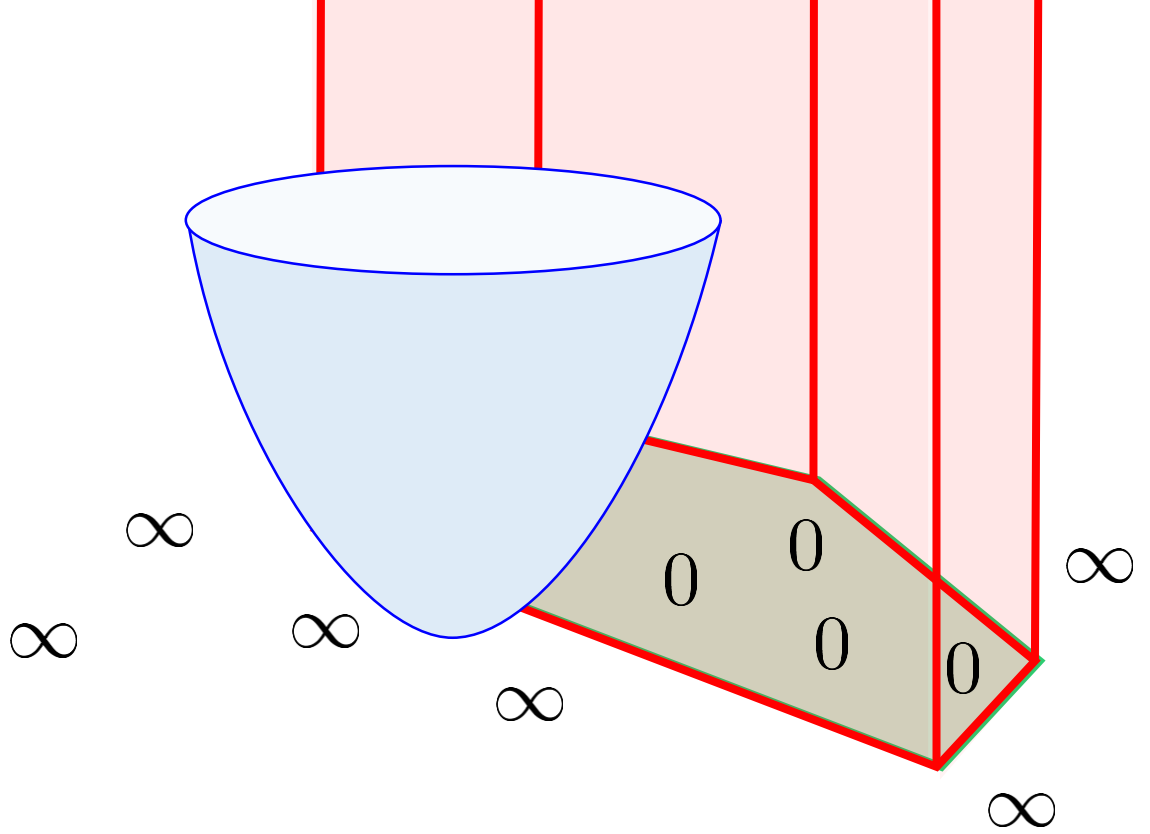

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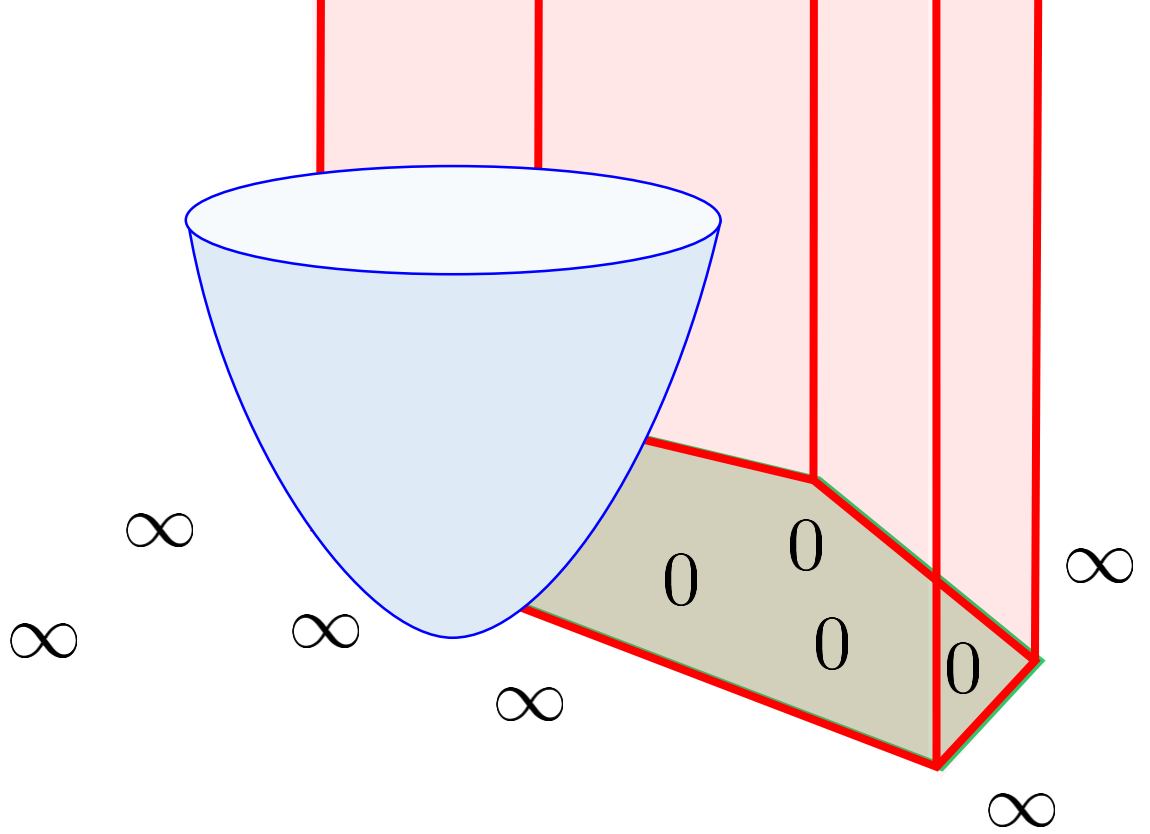

$$\hat{\mathbf{w}}_P = \arg\min_{\mathbf{w}\in\mathbb{R}^d} \{\arg\max_{\alpha\geq 0} \{\mathcal{L}(\mathbf{w},\alpha)\}\}$$

Primal problem

$$\hat{\mathbf{w}}_D = \arg\max_{\alpha\geq 0} \{\arg\min_{\mathbf{w}\in\mathbb{R}^d} \{\mathcal{L}(\mathbf{w},\alpha)\}\}$$

The Lagrangian

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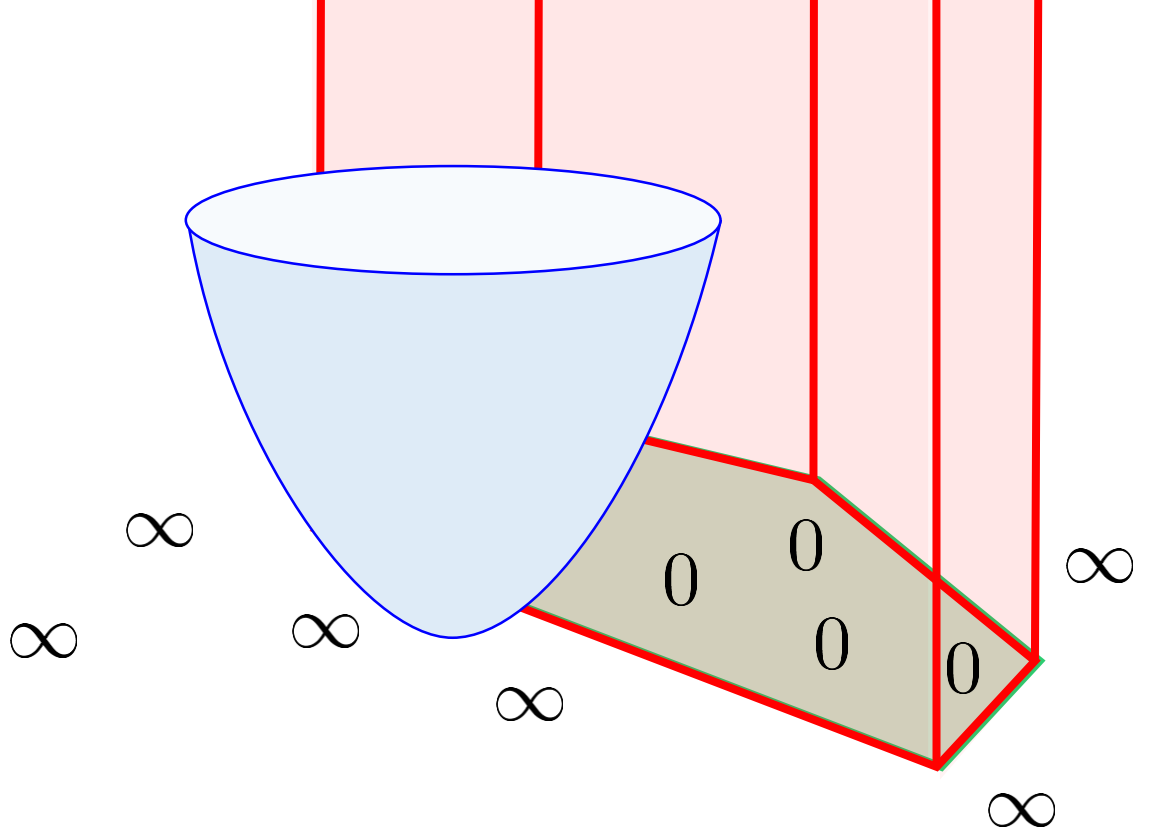
Primal problem



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Primal problem

$$\hat{\mathbf{w}}_D = \arg\max_{\alpha\geq 0} \{\arg\min_{\mathbf{w}\in\mathbb{R}^d} \{\mathcal{L}(\mathbf{w},\alpha)\}\}$$

Dual problem

The Lagrange Dual Problem

$$\hat{\mathbf{w}}_{\mathrm{P}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\arg\min}\ f(\mathbf{w})$$

$$\text{s.t. } g(\mathbf{w}) \leq 0$$

The Lagrange Dual Problem

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The Lagrange Dual Problem

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$$\hat{\mathbf{w}}_{\mathrm{D}} = \underset{\alpha \geq 0}{\arg\max} \left\{ \underset{\mathbf{w} \in \mathbb{R}^d}{\arg\min} \left\{ \mathcal{L}(\mathbf{w}, \alpha) \right\} \right\}$$

The Lagrange Dual Problem

$$\hat{\mathbf{w}}_{\mathrm{P}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w})$$

$$\text{s.t. } g(\mathbf{w}) \leq 0$$

$$\hat{\mathbf{w}}_{\mathrm{P}} \overset{?}{=} \hat{\mathbf{w}}_{\mathrm{D}}$$

$$\mathcal{L}(\mathbf{w}, \alpha) = f(\mathbf{w}) + \alpha \cdot g(\mathbf{w})$$

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$\hat{\mathbf{w}}_p = \hat{\mathbf{w}}_d$ for nice problems*

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E.g. if $f(\cdot)$ is convex and $\{\mathbf{w} : g(\mathbf{w}) \leq 0\}$ is convex

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$$\alpha_{\mathrm{D}} \cdot g(\hat{\mathbf{w}}_{\mathrm{D}}) = 0$$

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The maximizer

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The maximizer

Complimentary slackness KKT Condition

Multiple Constraints!

Multiple Constraints!

$$\hat{\mathbf{w}}_{\mathrm{P}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\arg\min}\ f(\mathbf{w})$$

$$\text{s.t. } g_1(\mathbf{w}) \leq 0, g_2(\mathbf{w}) \leq 0$$

$$h(\mathbf{w}) = 0$$

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$$\hat{\mathbf{w}}_{\mathrm{P}} = \underset{\mathbf{w}\in\mathbb{R}^d}{\arg\min}\ \{\underset{\substack{\alpha,\beta\geq 0\\ \gamma\in\mathbb{R}}}{\arg\max}\ \{f(\mathbf{w}) + \alpha \cdot g_1(\mathbf{w}) + \beta \cdot g_2(\mathbf{w}) + \gamma \cdot h(\mathbf{w})\}\}$$

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$$\text{s.t. } g_1(\mathbf{w}) \leq 0, g_2(\mathbf{w}) \leq 0$$

$$h(\mathbf{w}) = 0$$

One Lagrange multiplier for each constraint

$$\hat{\mathbf{w}}_{\mathrm{P}} = \arg\min_{\mathbf{w}\in\mathbb{R}^d} \{\arg\max_{\substack{\alpha,\beta\geq 0\\ \gamma\in\mathbb{R}}} \{f(\mathbf{w}) + \alpha \cdot g_1(\mathbf{w}) + \beta \cdot g_2(\mathbf{w}) + \gamma \cdot h(\mathbf{w})\}\}$$

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Doesn't allow $g_1(\mathbf{w}) > 0$

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Doesn't allow $g_1(\mathbf{w}) > 0$

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Multiple Constraints!

$$\hat{\mathbf{w}}_P = \arg\min_{\mathbf{w}\in\mathbb{R}^d} f(\mathbf{w})$$

Complimentary Slackness

$$\alpha_D \cdot g_1(\hat{\mathbf{w}}_D) = 0$$
$$\beta_D \cdot g_2(\hat{\mathbf{w}}_D) = 0$$
$$\gamma_D \cdot h(\hat{\mathbf{w}}_D) = 0$$

One Lagrange multiplier for each constraint

$$\text{s.t. } g_1(\mathbf{w}) \leq 0, g_2(\mathbf{w}) \leq 0$$
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$$\hat{\mathbf{w}}_D = \arg\max_{\substack{\alpha,\beta\geq 0\\ \gamma\in\mathbb{R}}} \{\arg\min_{\mathbf{w}\in\mathbb{R}^d} \{f(\mathbf{w}) + \alpha \cdot g_1(\mathbf{w}) + \beta \cdot g_2(\mathbf{w}) + \gamma \cdot h(\mathbf{w})\}\}$$

SVM Revisited

SVM Revisited

$$\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|_2^2$$

$$\text{s.t. } y^i \left\langle \mathbf{w}, \mathbf{x}^i \right\rangle \geq 1$$

SVM Revisited

$$\widehat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|_2^2$$

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n constraints, so n Lagrange multipliers

SVM Revisited

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n constraints, so n Lagrange multipliers

$\boldsymbol{\alpha} \in \mathbb{R}^n$

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$\boldsymbol{\alpha} \geq 0$ is notation for $\boldsymbol{\alpha}_i \geq 0$ for all i

SVM Revisited

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Inner problem is an Unconstrained problem so Gradients must vanish at optimum

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Optimal model $\hat{\mathbf{w}}$ is a weighted sum of training points!

SVM Revisited

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Points with $\boldsymbol{\alpha}_i \neq 0$ support vectors

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Lets substitute $\mathbf{w}$ in $\mathcal{L}$ and eliminate it!

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$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \boldsymbol{\alpha}_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \boldsymbol{\alpha}_i \boldsymbol{\alpha}_j y^i y^j \left\langle \mathbf{x}^i, \mathbf{x}^j \right\rangle$$

$$\hat{\mathbf{w}} = \hat{\mathbf{w}}_{\mathrm{D}} = \max_{\boldsymbol{\alpha} \geq 0} \left\{ \min_{\mathbf{w}} \ \mathcal{L}(\mathbf{w}, \boldsymbol{\alpha}) \right\}$$

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$$\hat{\boldsymbol{\alpha}} = \arg\max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \sum_{i=1}^{n} \boldsymbol{\alpha}_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \boldsymbol{\alpha}_i \boldsymbol{\alpha}_j y^i y^j \left\langle \mathbf{x}^i, \mathbf{x}^j \right\rangle$$

$$\text{s.t. } \boldsymbol{\alpha}_i \geq 0$$

SVM Revisited

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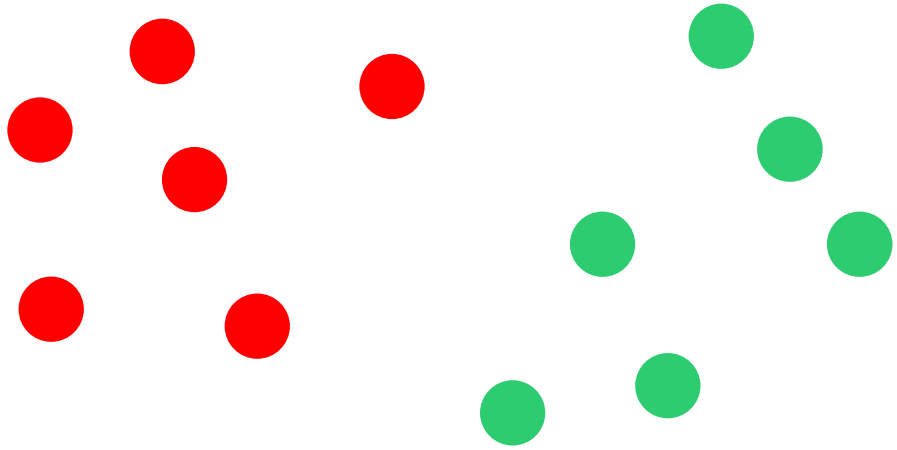

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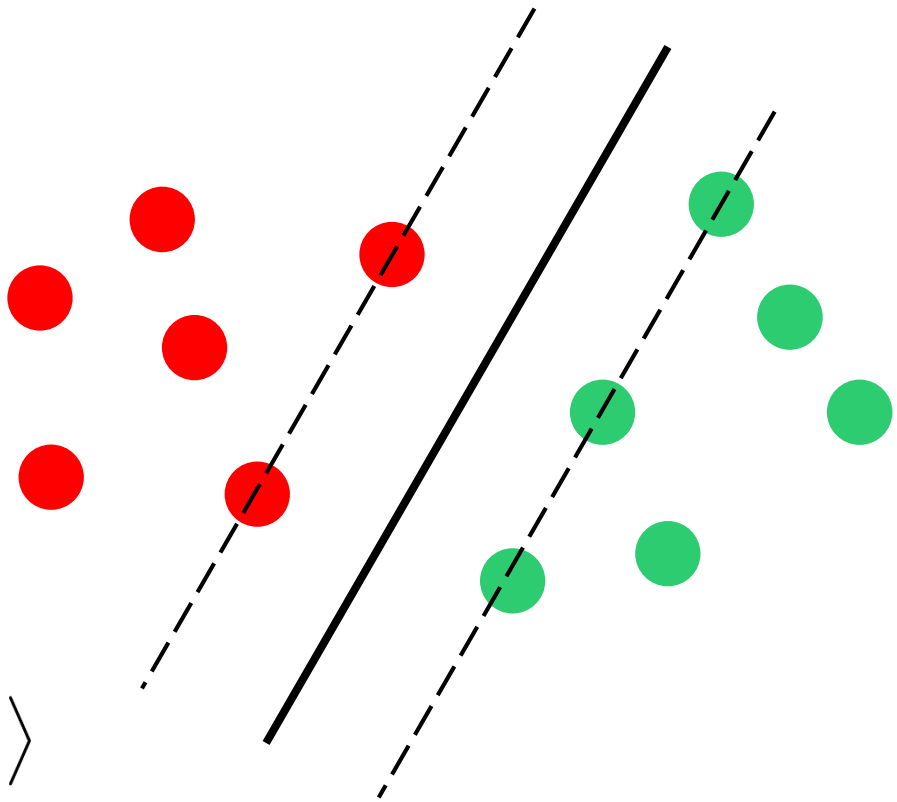

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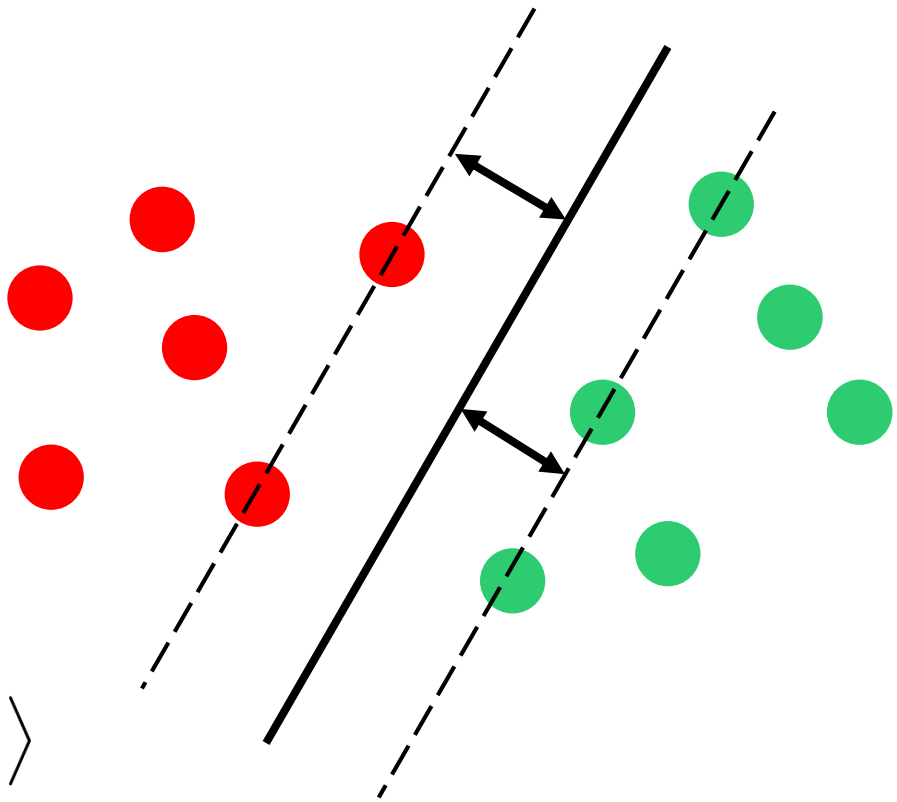

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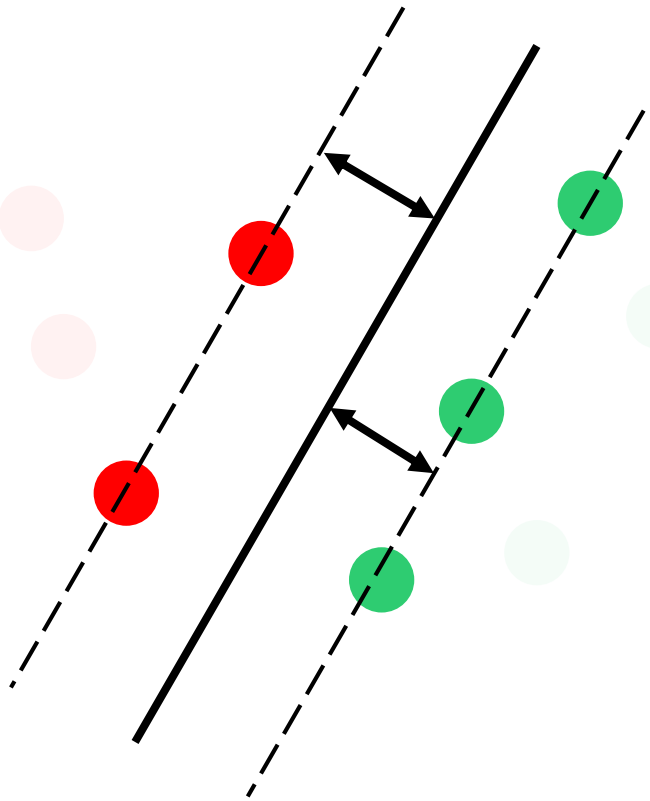

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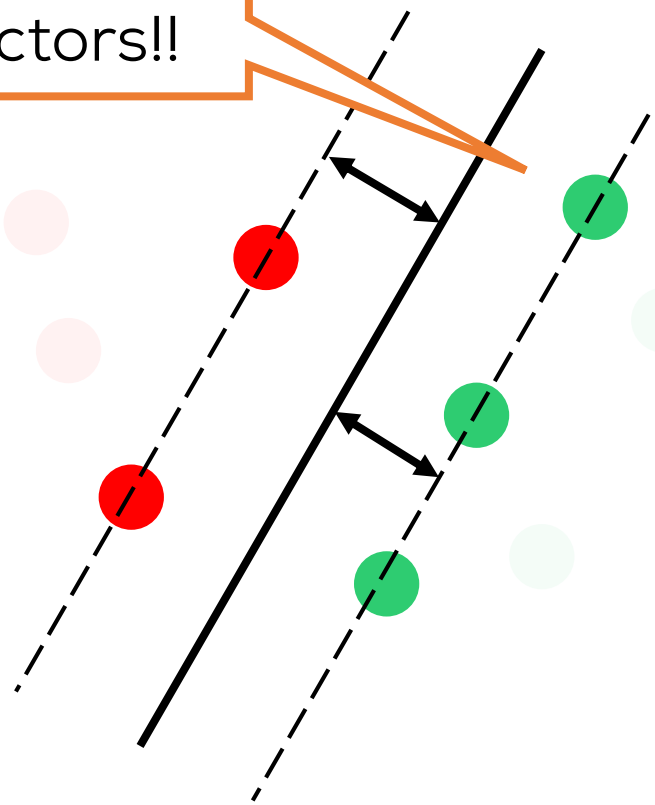

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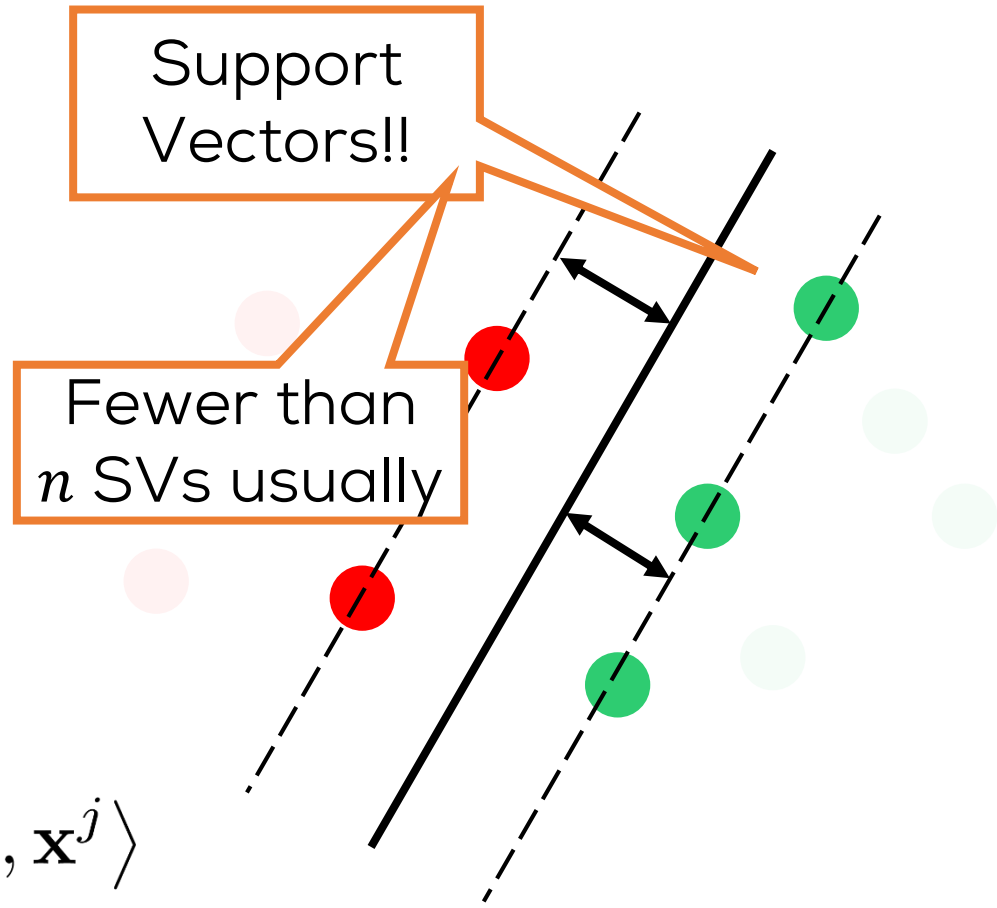

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Fewer than n SVs usually

$\|\boldsymbol{\alpha}\|_1$ is a sparsity promoting reg.!!

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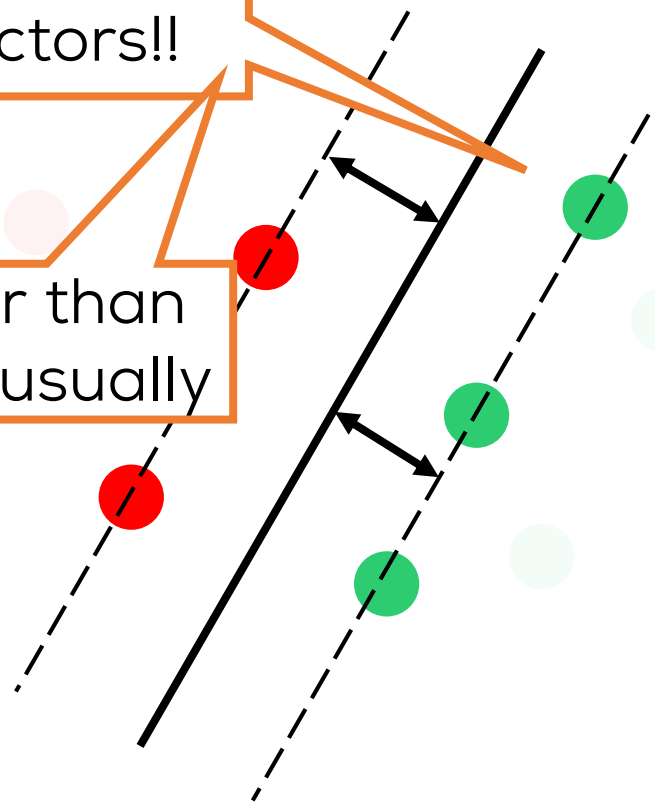

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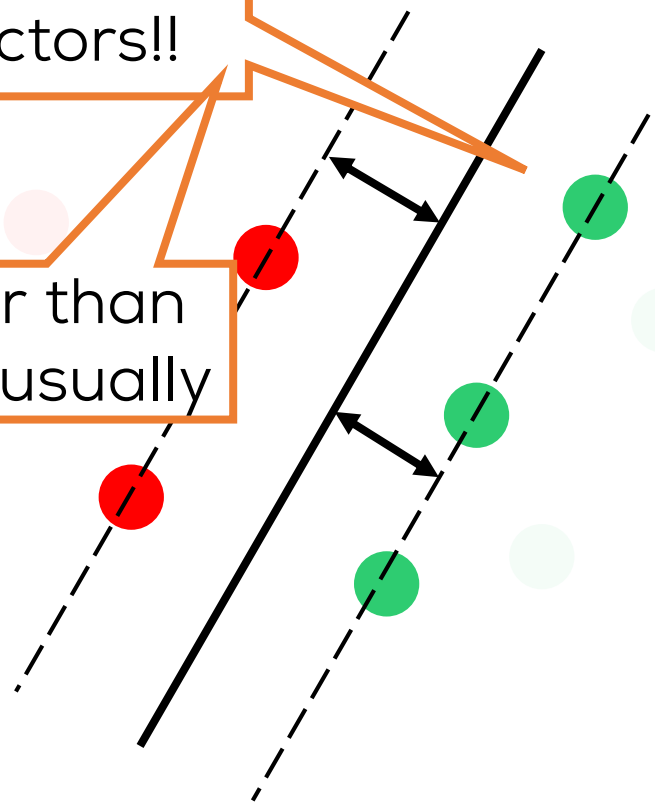

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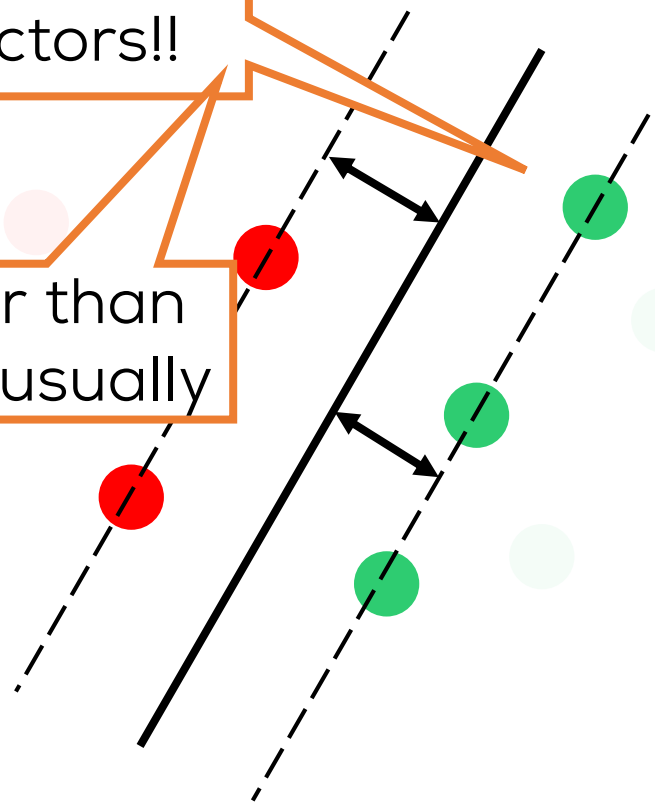

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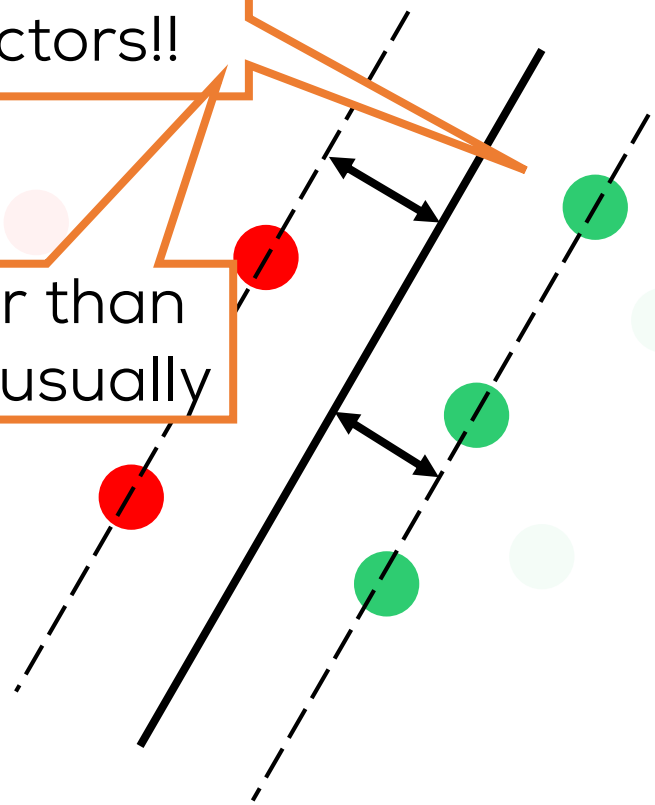

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Exercise

App: SVMs via CD

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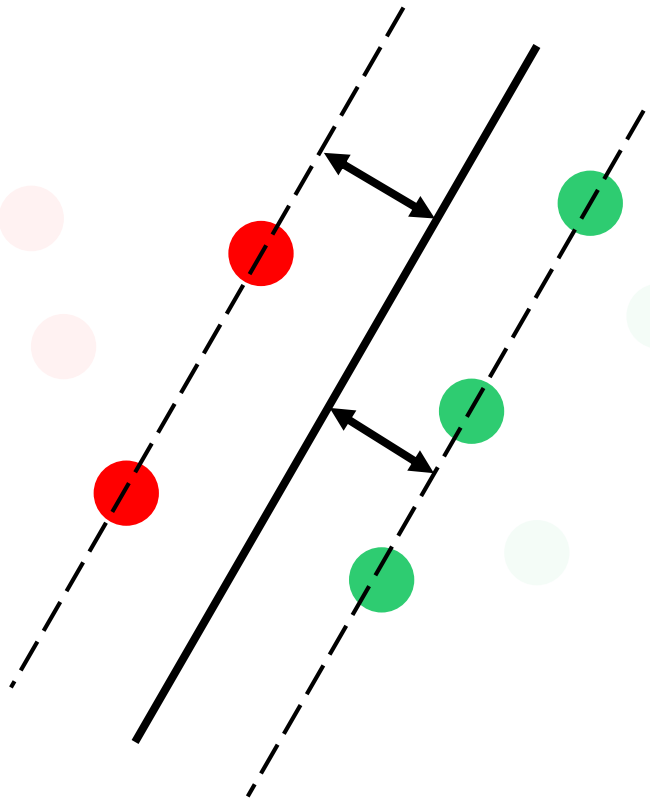

Coordinate Descent

- Similar to gradient descent except update one variable at a time
- Notation: $\nabla_i f(\mathbf{w}) = [\nabla f(\mathbf{w})]_\mathrm{i}$ i.e. the i-th directional derivative

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \; f(\mathbf{w}) + r(\mathbf{w})$$

COORDINATE DESCENT

1. Initialize $\mathbf{w}^0 \in \mathbb{R}^d$
2. Select a coordinate $j_t \in [d]$
3. Let $\mathbf{g}_{j_t}^t \leftarrow \nabla_{\mathrm{j_t}} f(\mathbf{w}^t) + \nabla_{\mathrm{j_t}} r(\mathbf{w}^t) \in \mathbb{R}$
4. Update $\mathbf{w}_{j_t}^{t+1} \leftarrow \mathbf{w}_{j_t}^t - \eta_t \cdot \mathbf{g}_{j_t}^t$
5. Preserve other coord. $\mathbf{w}_k^{t+1} \leftarrow \mathbf{w}_k^t,\ k \neq j_t$
6. Repeat until convergence

Random (Stochastic CD), Cyclic $1,2,\ldots,d,1,2,3\ldots d,\ldots$

Only $O(n)$ time per iter!

App: SVMs via CD

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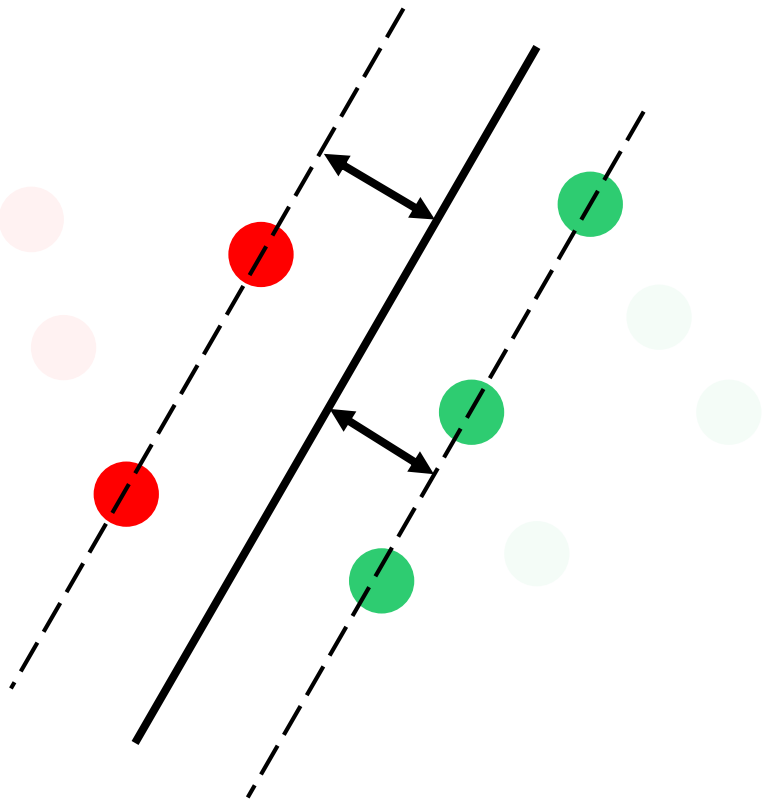

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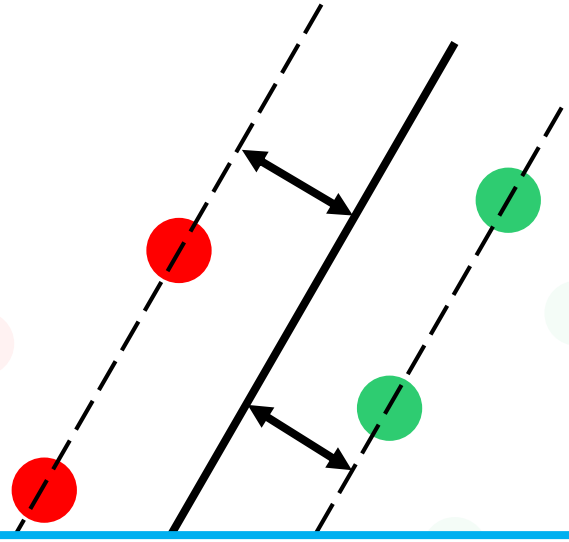

- Choose $i_t \in [n]$ at each time step (random, cyclic etc)
- Update only $\boldsymbol{\alpha}_{i_t}$, leave all other $\boldsymbol{\alpha}_i, \mathrm{i} \neq i_t$ untouched
  - Use projected gradient descent –constraint is pretty simple
- Note: $\boldsymbol{\alpha}_{i_t}$ corresponds to the data point $\left(\mathbf{x}^{i_t}, y^{i_t}\right)$
  - Only the i_t-th data point required to perform this update - exercise
  - Stochastic CD in dual looks like stochastic GD in primal!
- Current state of the art for SVMs – Liblinear, Scikit-learn

On to Data Modelling!

Hope you had fun with FA

Will revisit this method soon

For now, back to PML …

Please give your Feedback

http://tinyurl.com/ml17-18afb