

Convex Optimisation with the Alternating Directed Method of Multipliers Algorithm

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Overview

Background

Primal-Dual Optimality

Alternating Directed Method of Multipliers

Example: Piecewise Approximation

Summary

Background

Convex Optimisation¹

We consider an optimisation problem

$$\begin{aligned} & \min_{\theta} f(\theta) \\ & \text{s.t. } g(\theta) \leq 0 \end{aligned}$$

to be convex if $f: \mathbb{R}^p \mapsto \mathbb{R}$, $g: \mathbb{R}^p \mapsto \mathbb{R}^q$ are convex functions:

- Recall function is convex if

$$f(\alpha x + \beta y) \leq \alpha f(x) + \beta f(y)$$

for all $\alpha + \beta = 1$, $\alpha \geq 0, \beta \geq 0$ and $x, y \in \mathbb{R}^p$.

- We define the feasible set $\mathcal{F} := \{\theta \mid g(\theta) \leq 0\}$
- Define θ_* to be a minimiser of the above problem

¹See Convex Optimization by Boyd and Vandenberghe (esp. chapters 3, 5)
Background

Global vs Local Optimisation

► Global methods:

- Find the optimal θ_* over all feasible points in \mathcal{F}
- Worst case complexity grows exponentially with p, q

► Local methods:

- Find an optimal $\tilde{\theta}_*$ among feasible points that are deemed local.
- We could define locality as points close to some neighbourhood of a starting point $\mathcal{F} \cup \mathcal{N}(\theta_0)$

Benefits of Convex Optimisation

Convexity gives us conditions for finding global optima:

- ▶ Strict convexity implies there is a unique θ_*
- ▶ Generally, we may have an equivalence class $\mathcal{F}_* \subset \mathcal{F}$, such that

$$f(\theta_* \in \mathcal{F}_*) < f(\theta \in \mathcal{F} \setminus \mathcal{F}_*)$$

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Convex approximations (relaxations) can be useful as:

- ▶ Heuristics for Non-Convex problems (\implies approximate solutions)
- ▶ A way to initialize complex non-convex problems, find a good starting point \implies finding a good local minima?

Approach (for today)

- ▶ As formulated so far, we have both an objective to minimise, as well as constraints to consider.
- ▶ **Strategy:**
 - We will introduce some additional penalties, so that if we violate the constraints, a cost is added to the objective (i.e. the Lagrangian)
 - We can examine the saddle points of this augmented objective function
 - We will see that this gives rise to a related optimisation problem that is convex, even when the original problem is non-convex (weak-duality)

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 - We can examine the saddle points of this augmented objective function
 - We will see that this gives rise to a related optimisation problem that is convex, even when the original problem is non-convex (weak-duality)
 - ADMM is a structured way to solve this related problem (and also the original problem on the way).

Lagrangian

- We define the “primal” problem as

$$\begin{aligned} & \min_{\theta} f(\theta) \\ \text{s.t. } & g(\theta) \leq 0 \\ & h(\theta) = 0, \end{aligned}$$

where $g(\cdot) \mapsto \mathbb{R}^q$, $h(\cdot) \mapsto \mathbb{R}^r$, and comparison is entrywise².

²For a convex problem we require $h(\theta)$ is affine, e.g. can be written

$$h(\theta) = \langle a, \theta \rangle - b.$$

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- We define the *Lagrangian* as:

$$L(\theta, v, v_e) := f(\theta) + \langle v, g(\theta) \rangle + \langle v_e, h(\theta) \rangle$$

where $v \in \mathbb{R}^q$, $v_e \in \mathbb{R}^r$ are referred to as *Lagrange multipliers*.

²For a convex problem we require $h(\theta)$ is affine, e.g. can be written

$h(\theta) = \langle a, \theta \rangle - b$.

Conjugate Function

The conjugate function $f^*(y)$ of $f(x)$ is defined as

$$f^*(y) := \sup_{x \in \text{dom}(f)} \langle y, x \rangle - f(x)$$

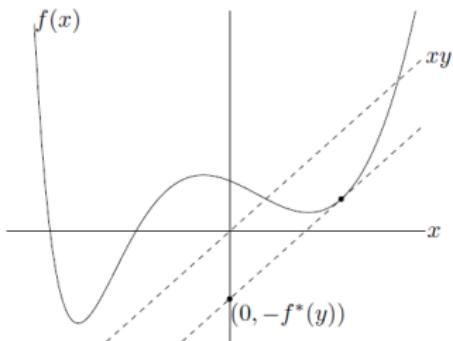


Figure 3.8 A function $f : \mathbb{R} \rightarrow \mathbb{R}$, and a value $y \in \mathbb{R}$. The conjugate function $f^*(y)$ is the maximum gap between the linear function yx and $f(x)$, as shown by the dashed line in the figure. If f is differentiable, this occurs at a point x where $f'(x) = y$.

Non-Convex \rightarrow Convex

The conjugate function f^* is convex, even if f is not:

- ▶ This follows from definition, as a point-wise supremum over a family of affine (convex) functions.
- ▶ Taking this supremum preserves the convexity of the affine function.

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When we work with the Lagrangian, we can be interested in seeing what the minimiser looks like as a function of the multipliers. This is defined as the dual function:

$$\begin{aligned} g(v, v_e) &= \inf_{\theta} L(\theta, v, v_e) \\ &= \inf_{\theta} \left(f(\theta) + \langle v, g(\theta) \rangle + \langle v_e, h(\theta) \rangle \right) \end{aligned}$$

- ▶ $g()$ is a point-wise infimum of affine functions, so is thus concave
- ▶ this is true even when $f()$ is not convex

Non-Convex → Convex

The dual, and conjugate functions are closely related. For example, consider

$$\min f(\theta) \quad s.t. \theta = 0.$$

We have³

$$\begin{aligned} L(\theta, v_e) &= f(\theta) + \langle v_e, \theta \rangle \\ g(v_e) &:= \inf_{\theta} [f(\theta) + \langle v_e, \theta \rangle] \\ &= -\sup_{\theta} [\langle -v_e, \theta \rangle - f(\theta)] \\ &= -f^*(-v_e). \end{aligned}$$

³Recall the conjugate is defined as $f^*(\beta) := \sup_{\theta \in \text{dom}(f)} \langle \beta, \theta \rangle - f(\theta)$.
Background

Non-Convex \rightarrow Convex

More generally, we may have

$$\begin{aligned} & \min f(\theta) \\ \text{s.t. } & A\theta \leq a \\ & B\theta = b \end{aligned}$$

And thus⁴

$$\begin{aligned} L(\theta, v_e) &= f(\theta) + \langle v, A\theta - a \rangle + \langle v_e, B\theta - b \rangle \\ g(v_e) &:= \inf_{\theta} [f(\theta) + \langle v, A\theta - a \rangle + \langle v_e, B\theta - b \rangle] \\ &= -a^T v - b^T v_e + \inf_{\theta} [f(\theta) + (A^T v + B^T v_e)^T \theta] \\ &= -a^T v - b^T v_e - f^*(-A^T v - B^T v_e) \end{aligned}$$

⁴Recall the conjugate is defined as $f^*(\beta) := \sup_{\theta \in \text{dom}(f)} \langle \beta, \theta \rangle - f(\theta)$.

Primal-Dual Optimality

Lagrange Dual Problem

The dual function traces out the optimal value of the objective, as a function of the multipliers. Now, which value of multipliers is the best?

- ▶ This is known as the *Lagrangian Dual Problem*:

$$\begin{aligned} & \max g(v, v_e) \\ & \text{s.t. } v \geq 0 \end{aligned} \tag{1}$$

- ▶ We define a *dual-feasible pair*, as (v, v_e) , such that for $v \geq 0$ we have $g(v, v_e) > -\infty$, i.e. v is feasible for the dual problem above.
- ▶ Define the *dual optimal pair* (v^*, v_e^*) as the solution (maximiser) of (1)

Weak Duality

Let us define the optimal value of the dual problem and the primal problem

$$\begin{aligned}\mathcal{D} &= g(v^*, v_e^*) \\ \mathcal{P} &= f(\theta^*) .\end{aligned}$$

Then we have (even if the original problem is non-convex), that

$$\mathcal{D} \leq \mathcal{P} .$$

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Consequences:

- ▶ If primal problem is unbounded below such that $\mathcal{P} = -\infty$, then we have $\mathcal{D} = -\infty$
- ▶ If dual problem is unbounded above $\mathcal{D} = \infty$, then we also have $\mathcal{P} = \infty$ (which implies the primal problem is infeasible).

Verification

The fact $\mathcal{D} \leq \mathcal{P}$ can be easily verified:

- ▶ Let $\tilde{\theta} \in \mathcal{F}$ be a feasible point, i.e. $g(\tilde{\theta}) \leq 0$ and $h(\tilde{\theta}) = 0$
- ▶ This gives us the additional cost

$$\underbrace{\langle v, g(\tilde{\theta}) \rangle}_{\leq 0} + \underbrace{\langle v_e, h(\tilde{\theta}) \rangle}_{= 0} \leq 0,$$

where we remember we have $v \geq 0$.

- ▶ Thus we have $L(\tilde{\theta}, v, v_e) \leq f(\tilde{\theta})$, for any $\tilde{\theta} \in \mathcal{F}$, and we recall $\theta_* \in \mathcal{F}$.

Strong Duality

We refer to the difference $\text{gap} := \mathcal{P} - \mathcal{D} \geq 0$ as the *optimal duality gap*.

- ▶ If the primal problem is convex, then we usually have $\text{gap} = 0$
- ▶ If we have $\text{gap} = 0$ for a problem, then we say *strong-duality* holds.

⁵See Boyd Section 5.2. for examples and discussion.

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Conditions under which we have strong-duality are known as *constraint qualifications*.

- ▶ If the conditions are met, then we can try to solve the dual problem, to solve the primal.
- ▶ Otherwise, solving the dual, can lower-bound the primal.
- ▶ Such conditions exist even for some (specific) non-convex problems⁵.

⁵See Boyd Section 5.2. for examples and discussion.

Min-Max \iff Max-Min

- ▶ Consider the definition of the optimal values

$$\mathcal{P} = \inf_{\theta} \sup_{v \geq 0} L(\theta, v)$$

$$\mathcal{D} = \sup_{v \geq 0} \inf_{\theta} L(\theta, v)$$

- ▶ Then

$$\mathcal{D} \leq \mathcal{P} \implies \sup_{v \geq 0} \inf_{\theta} L(\theta, v) \leq \inf_{\theta} \sup_{v \geq 0} L(\theta, v)$$

- ▶ Strong-duality gives us

$$\sup_{v \geq 0} \inf_{\theta} L(\theta, v) = \inf_{\theta} \sup_{v \geq 0} L(\theta, v) .$$

Alternating Directed Method of Multipliers

Motivation⁶

Depending on the structure within the primal problem, solving the dual-problem may or may not be easier than the primal.

- ▶ We will focus on algorithms which iteratively try to solve the problem

$$\inf_{\theta} \sup_{v \geq 0} L(\theta, v) \implies \theta^* = \arg \min_{\theta} L(\theta, v^*) \quad (2)$$

- ▶ That is, we try a sequence of θ^k, v^k such that as $k \rightarrow \infty$ we have $\theta^k, v^k \rightarrow \theta^*, v^*$
- ▶ We assume strong-duality, so that we can use the implication (2).
- ▶ *We limit ourselves to convex problems*

⁶Recommend the review article by Boyd et al. "Distributed optimization and statistical learning via the alternating direction method of multipliers", 2011

Dual Ascent

- ▶ Consider the equality constrained optimization

$$\begin{aligned} & \min f(\theta) \\ \text{s.t. } & A\theta = a . \end{aligned}$$

- ▶ Assume that the dual $g(v)$ is differentiable, then letting

$$\theta' = \arg \min_{\theta} L(\theta, v) ,$$

gives us $\nabla g(v) = A\theta' - a$.

- ▶ This motivates a simple “algorithm” for finding the maximisers by iterating

$$\begin{aligned} \theta^{k+1} &= \arg \min_{\theta} L(\theta, v^k) \\ v^{k+1} &= v^k + \alpha(A\theta^{k+1} - a) \end{aligned}$$

where $\alpha > 0$ is a step-size parameter.

Separability

- We will be particularly interested in the case where $f(\theta)$ is *linearly separable*, i.e.

$$f(\theta) = \sum_{i=1}^m f_i(\theta).$$

- The equality constraint can also be partitioned $A = [A_1, \dots, A_m]$ such that $A\theta = \sum_{i=1}^m A_i\theta_i$.

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- The Lagrangian can then be written as

$$L(\theta, v) = \sum_{i=1}^m \left[f_i(\theta_i) + \langle v, A_i \theta_i \rangle - \frac{1}{m} \langle v, a \rangle \right].$$

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- This permits the splitting of the minimisation step, over $\{\theta_i\}_{i=1}^m$ as:

$$\theta_i^{k+1} = \arg \min_{\theta_i} L_i(\theta_i, v^k)$$

$$v^{k+1} = v^k + \alpha(A\theta^{k+1} - a)$$

Augmented Lagrangian

In order to enable convergence without strict convexity assumptions (or finiteness of f), researchers turned to the Augmented Lagrangian

$$L_\rho(\theta, v) = f(\theta) + \langle v, A\theta - a \rangle + \frac{\rho}{2} \|A\theta - a\|_2^2.$$

- ▶ This adds curvature around the equality constraint $A\theta \approx a$
- ▶ $\rho > 0$ impacts the level of curvature added.
- ▶ Define the augmented dual as $g_\rho(v) := \inf_\theta L(\theta, v)$.

⁷The step-size ρ can be motivated through looking at the optimality (primal and dual feasibility) conditions and relating the update v^{k+1} with the previous step v^k , see e.g. p12 Boyd.

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- ▶ $\rho > 0$ impacts the level of curvature added.
- ▶ Define the augmented dual as $g_\rho(v) := \inf_\theta L(\theta, v)$.
- ▶ The *Method of Multipliers* algorithm is simply Lagrangian ascent applied to $g_\rho(v)$ ⁷

$$\theta^{k+1} = \arg \min_{\theta} L_\rho(\theta_i, v^k)$$

$$v^{k+1} = v^k + \rho(A\theta^{k+1} - a)$$

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Alternating Directed Method of Multipliers

We now consider the setting where the objective is separable, and the equality constraint links these components, i.e.

$$\begin{aligned} & \min_{\theta, \beta} f_A(\theta) + f_B(\beta) \\ & \text{s.t. } A\theta + B\beta = c \end{aligned}$$

- The linear equality constraints allow us to let β be a linear transformation of θ .

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- ▶ E.g. In statistics, $-f_A(\theta)$ may be a (log)likelihood and $-f_B(T\theta)$ may be a log-prior, which leads to the minimiser being equivalent to the MAP.

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- ▶ E.g. In statistics, $-f_A(\theta)$ may be a (log)likelihood and $-f_B(T\theta)$ may be a log-prior, which leads to the minimiser being equivalent to the MAP.
- ▶ This also allows for the block-seperability as before, e.g. if $f(\theta) = \sum_i f_i(\theta_i)$

Alternating Directed Method of Multipliers

Let us write the augmented Lagrangian, and then consider the method of multipliers

$$L_\rho(\theta, \beta, v) = f_A(\theta) + f_B(\beta) + \underbrace{\langle v, A\theta + B\beta - c \rangle}_{=: \text{res}} + \frac{\rho}{2} \|A\theta + B\beta - c\|_2^2.$$

Given the separability of $f_A(\theta)$ and $f_B(\beta)$, we can consider $\arg \min_{(\theta, \beta)} L_\rho(\theta, \beta, v)$ in two distinct updates

$$\theta^{k+1} = \arg \min_{\theta} L_\rho(\theta, \beta^k, v^k)$$

$$\beta^{k+1} = \arg \min_{\beta} L_\rho(\theta^{k+1}, \beta, v^k)$$

$$v^{k+1} = v^k + \rho \underbrace{(A\theta^{k+1} + B\beta^{k+1} - a)}_{=: r^k}$$

Convergence (Theory)

Convergence of the iterates θ^k, β^k, v^k is guaranteed under relatively assumptions:

1. $f : \mathbb{R}^p \mapsto \mathbb{R} \cup \{+\infty\}$, $g : \mathbb{R}^q \mapsto \mathbb{R} \cup \{+\infty\}$ are closed, proper and convex.⁸
2. There exists (θ^*, β^*, v^*) such that L_0 has a saddle point

$$L_0(\theta^*, \beta^*, v) \leq L(\theta^*, \beta^*, v^*) \leq L(\theta, \beta, v^*)$$

From which we obtain, $k \rightarrow \infty$:

- Residual convergence, $r^k \rightarrow 0$.
- Objective convergence, $f_A(\theta^k) + f_B(\beta^k) \rightarrow \mathcal{P}$
- Dual convergence, $v^k \rightarrow v^*$, where v^* is a dual optimal point.

Further results are available under additional assumptions.⁹

⁸Implied iff the epigraphs, e.g. $\text{epi}(f)$ are closed and non-empty sets.

⁹See e.g. Wang 2019, *Global Convergence of ADMM in Nonconvex Nonsmooth Optimization*. Hong et al. 2017, *On the Linear Convergence of the Alternating Direction Method of Multipliers*.

Convergence (in practice)

The practical rate of convergence for ADMM varies on the application.

- ▶ This can be sensitive to the specification of $\rho \geq 0$.
- ▶ Some work considers adaptive step-size schemes where $\{\rho_k\}$ is a decreasing sequence.
- ▶ Usually, can converge to reasonable solutions in a few iterations (10's), but slow to converge to high-precision.

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It is worth to consider also the positives:

- ▶ Can easily be parallelised in the case that the θ^{k+1} or β^{k+1} updates are separable.
- ▶ Often, for popular choices of $f_A()$, $f_B()$ we may have closed form (efficient) solutions for the sub-problems (low iteration complexity).

Example: Piecewise Approximation

Trend-Filtering

- ▶ As a simple example, we will consider a variant of the “fused-Lasso”.
- ▶ Basically, an ℓ_2 least-squares objective, with a penalty enforcing smoothness on the variation of the mean.
- ▶ Consider the model for time points $t = 1, \dots, n$

$$y_t = \theta_t + \varepsilon_t \quad ; \quad \varepsilon_t \sim \mathcal{N}(0, \sigma^2)$$

$$\text{s.t.} \quad \sum_{t=2}^n |\theta_t - \theta_{t-1}| \leq \eta$$

and $\eta \geq 0$ represents a constraint on the variation of $\mathbb{E}[y_t] = \theta_t$.

Estimator (ℓ_1 -Trend Filter)

We consider a penalised MLE

$$\arg \min_{\theta, \beta} \left[\underbrace{\frac{1}{2n} \|y - \theta\|_2^2}_{f_A(\theta)} + \underbrace{\lambda \|\beta\|_1}_{f_B(\beta)} \right]$$

s.t. $\beta = D\theta$,

where $D \in \mathbb{R}^{n-1 \times n}$ is a differencing matrix.

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where $D \in \mathbb{R}^{n-1 \times n}$ is a differencing matrix.

Write the augmented Lagrangian problem

$$\arg \min_{A\theta + B\beta = c} \max_{v \in \mathbb{R}^n} \left[f_A(\theta) + f_B(\beta) + \langle v, \text{res} \rangle + \frac{\rho}{2} \|\text{res}\|_2^2 \right]$$

where we choose $A = D$, $B = -I$, $c = 0$

ADMM (ℓ_1 -Trend Filter)

Recall the general problem

$$\arg \min_{A\theta + B\beta = c} \max_{v \in \mathbb{R}^n} \underbrace{\left[f_A(\theta) + f_B(\beta) + \langle v, \text{res} \rangle + \frac{\rho}{2} \|\text{res}\|_2^2 \right]}_{L_\rho(\theta, \beta, v)}$$

- With a simple rescaling, $\tilde{v} = v/\rho$ we can rewrite $L_\rho(\theta, \beta, v)$ as

$$\begin{aligned} L_\rho(\theta, \beta, v) &\equiv L_\rho(\theta, \beta, \tilde{v}) \\ &= f_A(\theta) + f_B(\beta) + \frac{\rho}{2} \|\text{res} + \tilde{v}\|_2^2 - \frac{\rho}{2} \|\tilde{v}\|_2^2 \end{aligned}$$

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- Now choosing $A = D$, $B = -I$, $c = 0$, and replacing v with \tilde{v} in our algorithm, we find

$$\theta^{k+1} = \arg \min_{\theta} L_\rho(\theta, \beta^k, \tilde{v}^k)$$

$$\beta^{k+1} = \arg \min_{\beta} L_\rho(\theta^{k+1}, \beta, \tilde{v}^k)$$

$$\tilde{v}^{k+1} = \tilde{v}^k + D\theta^{k+1} - \beta^{k+1}$$

ADMM (ℓ_1 -Trend Filter)

Let us consider the specific updates involved:

1. “Primal” update for $\theta^{k+1} = \arg \min_{\theta} L_p(\theta, \beta^k, \tilde{v}^k)$

$$\begin{aligned}\theta^{k+1} &= \arg \min_{\theta} \left[f_A(\theta) + \frac{\rho}{2} \|\text{res} + \tilde{v}^k\|_2^2 \right] \\ &= \arg \min_{\theta} \left[\frac{1}{2n} \|y - \theta\|_2^2 + \frac{\rho}{2} \|D\theta - \beta^{k+1} + \tilde{v}^k\|_2^2 \right] \\ &= (n^{-1} I_n + \rho D^\top D)^{-1} \left[\frac{y}{n} + \rho D^\top (\beta^k - \tilde{v}^k) \right]\end{aligned}$$

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$$\begin{aligned}\theta^{k+1} &= \arg \min_{\theta} \left[f_A(\theta) + \frac{\rho}{2} \|\text{res} + \tilde{v}^k\|_2^2 \right] \\ &= \arg \min_{\theta} \left[\frac{1}{2n} \|y - \theta\|_2^2 + \frac{\rho}{2} \|D\theta - \beta^{k+1} + \tilde{v}^k\|_2^2 \right] \\ &= (n^{-1} I_n + \rho D^\top D)^{-1} \left[\frac{y}{n} + \rho D^\top (\beta^k - \tilde{v}^k) \right]\end{aligned}$$

1. “Auxiliary” update for $\beta^{k+1} = \arg \min_{\beta} L_p(\theta^{k+1}, \beta, \tilde{v}^k)$:

$$\begin{aligned}\beta^{k+1} &= \arg \min_{\beta} \left[\lambda \|\beta\|_1 + \frac{\rho}{2} \|\text{res} + \tilde{v}^k\|_2^2 \right] \\ &= \arg \min_{\beta} \left[\frac{\rho}{2} \|D\theta^{k+1} + \tilde{v}^k - \beta\|_2^2 + \lambda \|\beta\|_1 \right] \\ &\equiv \text{prox}_{\frac{2\lambda}{\rho} \|\cdot\|_1} (D\theta^{k+1} + \tilde{v}^k) \\ &= \text{soft}(D\theta^{k+1} + \tilde{v}^k, 2\lambda/\rho)\end{aligned}$$

Summary

Conclusion

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- ▶ Idea, try to maximise the dual function to find a primal solution

Pros:

- ▶ Can easily make use of structure in common problems via known proximity operators
- ▶ Can be easily distributed/parallelised
- ▶ Guaranteed convergence under broad assumptions (convexity)
- ▶ Can be heuristically extended to allow for multiple blocks (e.g. multiple penalties)

Cons:

- ▶ Convergence rate is not necessarily great.
- ▶ Needs some thinking about how to split problem in most efficient way

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Thank you for listening!