Optimization for Statistics and Machine Learning

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What's Duality Good For?

Certify that your algorithm is correct

- duality gap and KKT conditions

Broaden your algorithm design menu

- You could solve the primal problem, but solving the dual problem takes less time to develop code, has better numerical properties, etc.

What's Duality Good For?

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Lagrangian

Standard form optimization problem (not necessarily convex)

$$\begin{aligned} \text{minimize } & f_0(x) \\ \text{subject to } & f_i \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{aligned}$$

where $x \in \mathbb{R}^n$, domain $\mathcal{D}$, and optimal value is $p^\star$.

Lagrangian: $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$, dom $\mathcal{L} = \mathcal{D} \times \mathbb{R}^m \times \mathbb{R}^p$,

$$\mathcal{L}(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

- weighted sum of objective and constraint functions
- $\lambda_i \geq 0$ is Lagrange multiplier associated with $f_i(x) \leq 0$
- ν_i is Lagrange multiplier associated with $h_i(x) = 0$

Relationship between Lagrangian and Primal Problem

$$\psi_P(x) = \sup_{\lambda \geq 0, \nu} \mathcal{L}(x, \lambda, \nu)$$

- "P" stands for "primal"
- If x violates any of the primal constraints ($f_i(x) > 0$ or $h_i(x) \neq 0$ for any i) then $\psi_P(x) = \infty$.
- If x satisfies the primal constraints then $\psi_P(x) = f_0(x)$

$$\psi_P(x) = \begin{cases} f_0(x) & \text{if } x \text{ is primal feasible} \\ \infty & \text{o.w.} \end{cases}$$

Equivalent unconstrained minimization

$$\inf_x \psi_P(x) = \inf_x \sup_{\lambda \geq 0, \nu} \mathcal{L}(x, \lambda, \nu)$$

Lagrangian Dual Function

Lagrange Dual Function: $\psi_D : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$ - "D" stands for "dual"

$$\psi_D(\lambda, \nu) = \inf_{x \in \mathcal{D}} \mathcal{L}(x, \lambda, \nu)$$

$$= \inf_{x \in \mathcal{D}} \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x) \right)$$

- ψ_D is concave, because it is the point-wise infimum of a collection of affine functions.

Lagrangian Dual Function

$$\psi_D(\lambda,\nu) = \inf_{x\in\mathcal{D}} \mathcal{L}(x,\lambda,\nu)$$
$$= \inf_{x\in\mathcal{D}} \left(f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x) \right)$$

lower bound property: if $\lambda \geq 0$, then $\psi_D(\lambda,\nu) \leq p^\star$
Proof: $\tilde{x}$ feasible $\implies \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x) \leq 0$

$$\psi_D(\lambda,\nu) \leq \mathcal{L}(\tilde{x},\lambda,\nu) \leq f_0(\tilde{x})$$

Since $\tilde{x}$ is an arbitrary feasible point, $\psi_D(\lambda,\nu) \leq p^\star$
Optimize lower bound:

$$\sup_{\lambda\geq 0,\nu} \psi_D(\lambda,\nu) = d^\star \leq p^\star$$

Least Euclidean norm solution to least squares

$$\text{minimize } b^T b$$

$$\text{subject to } X^T X b = X^T y$$

dual function

- $\mathcal{L}(b, \nu) = b^T b + \nu^T (X^T X b - X^T y)$
- Minimize $\mathcal{L}$ over b by setting gradient to zero

$$\nabla_b \mathcal{L}(b, \nu) = 2b + X^T X \nu = 0 \implies b = -(1/2) X^T X \nu$$

- Plug optimal b into $\mathcal{L}$ to get ψ_D:

$$\psi_D(\nu) = \mathcal{L}(-(1/2) X^T X \nu, \nu) = -\frac{1}{4} \nu^T (X^T X)^2 \nu - y^T X \nu$$

lower bound property says

$$p^\star \geq -\frac{1}{4} \nu^T (X^T X)^2 \nu - y^T X \nu,$$

for all ν.

Standard Form LP

$$\begin{aligned} &\text{minimize } c^T x \\ &\text{subject to } Ax = b, \quad x \geq 0 \end{aligned}$$

dual function

$$\begin{aligned} \mathcal{L}(x, \lambda, \nu) &= c^T x + \nu^T (Ax - b) - \lambda^T x \\ &= -b^T \nu + (c + A^T \nu - \lambda)^T x \end{aligned}$$

- $\mathcal{L}$ is affine in x

$$\psi_{\mathcal{D}}(\lambda, \nu) = \inf_x \mathcal{L}(x, \lambda, \nu) = \begin{cases} -b^T \nu & A^T \nu - \lambda + c = 0 \\ -\infty & \text{o.w.} \end{cases}$$

- $\psi_{\mathcal{D}}(\lambda, \nu)$ is linear on affine domain

$\{(\lambda, \nu) : A^T \nu - \lambda + c = 0\} \implies \psi_{\mathcal{D}}(\lambda, \nu)$ is concave.

lower bound property: $p^\star \geq -b^T \nu$ if $A^T \nu + c \geq 0$.

Lagrange Dual and Fenchel Conjugates

$$\begin{aligned} &\text{minimize } f_0(x) \\ &\text{subject to } Ax \leq b, \quad Cx = d \end{aligned}$$

dual function

$$\begin{aligned} \psi_D(\lambda, \nu) &= \inf_{x \in \mathbf{dom} f_0} \left[f_0(x) + (A^T\lambda + C^T\nu)^T x - b^T\lambda - d^T\nu \right] \\ &= -f_0^\star(-A^T\lambda - C^T\nu) - b^T\lambda - d^T\nu. \end{aligned}$$

Fenchel conjugate

$$f^\star(y) = \sup_{x \in \mathbf{dom} f} \; y^T x - f(x)$$

Quadratic Program

primal problem (assume $P \in S^n_{++}$)

$$\begin{aligned} &\text{minimize } x^T P x + q^T x \\ &\text{subject to } Ax \leq b, \quad Cx = d \end{aligned}$$

dual function

$$\begin{aligned} \psi_D(\lambda, \nu) &= -\frac{1}{4}\left[(z-q)^T P^{-1}(z-q)\right] - b^T\lambda - d^T\nu \\ z &= -A^T\lambda - C^T\nu \end{aligned}$$

The Dual Problem

Lagrange dual problem

$$\begin{aligned} &\text{maximize } \psi_D(\lambda, \nu) \\ &\text{subject to } \lambda \geq 0 \end{aligned}$$

- finds best possible lower bound on $p^\star$ that the Lagrange dual function can provide
- the dual problem is a convex optimization problem with optimal value $d^\star$
- λ, ν are dual feasible if $\lambda \geq 0, (\lambda, \nu) \in \text{dom}\psi_D$
- often simplified by making implicit constraint $(\lambda, \nu) \in \text{dom}\psi_D$ explicit

example: standard form LP and its dual

$$\begin{aligned} &\text{minimize } c^T x \\ &\text{subject to } Ax = b, \quad x \geq 0 \end{aligned}$$

$$\begin{aligned} &\text{maximize } -b^T \nu \\ &\text{subject to } A^T \nu + c \geq 0 \end{aligned}$$

Weak and Strong Duality

weak duality: $d^\star \leq p^\star$

- always holds (for convex and nonconvex programs)
- can be used to find nontrivial lower bounds for difficult problems

strong duality: $d^\star = p^\star$

- does not hold in general
- (usually) holds for convex problems
- conditions that guarantee strong duality in convex problems are called **constraint qualifications**

duality gap: (x, λ, ν)

$$\psi_P(x) - \psi_D(\lambda, \nu)$$

Slater's Constraint Qualification

strong duality holds for a convex problem

$$\begin{aligned} &\text{minimize } f_0(x) \\ &\text{subject to } f_i(x) \leq 0, \quad Ax = b \end{aligned}$$

if it is strictly feasible

$$\exists x \in \text{int}\mathcal{D} : f_i(x) < 0, \quad i = 1, \ldots, m, \quad Ax = b$$

- also guarantees that the dual optimum is attained (if $p^\star > -\infty$)
- can be sharpened: e.g. can replace int $\mathcal{D}$ with relint $\mathcal{D}$; linear inequalities do not need to hold with strict inequality, ...
- there are many other types of constraint qualifications

Inequality Form LP

primal problem

$$\begin{aligned} &\text{minimize } c^T x \\ &\text{subject to } Ax \leq b \end{aligned}$$

dual function

$$\psi_D(\lambda) = \inf_x \left((c + A^T\lambda)^T x - b^T\lambda \right) = \begin{cases} -b^T\lambda & A^T\lambda + c = 0 \\ -\infty & \text{o.w.} \end{cases}$$

dual problem

$$\begin{aligned} &\text{maximize } -b^T\nu \\ &\text{subject to } A^T\nu + c = 0 \end{aligned}$$

- from Slater's condition: $p^\star = d^\star$ if $A\tilde{x} < b$ for some $\tilde{x}$
- $p^\star = d^\star$ as long as either the primal or dual problem is feasible

Linear Programs and Duality Gap

Four possibilities:

- Primal optimal, dual optimal: $p^\star = d^\star$ (no gap)
- Primal unbounded, dual infeasible: $p^\star = d^\star = -\infty$ (no gap)
- Primal infeasible, dual unbounded: $p^\star = d^\star = \infty$ (no gap)
- Primal infeasible, dual infeasible: $p^\star = +\infty, d^\star = -\infty$ (infinite gap)

Quadratic Program

primal problem (assume $P \in S^n_{++}$)

$$\begin{array}{ll} \text{minimize} & x^T P x \\ \text{subject to} & Ax \leq b \end{array}$$

dual function

$$\psi_D(\lambda) = \inf_x \left(x^T P x + \lambda^T (Ax - b) \right) = -\frac{1}{4} \lambda^T A P^{-1} A^T \lambda - b^T \lambda$$

dual problem

$$\begin{array}{ll} \text{maximize} & -\frac{1}{4} \lambda^T A P^{-1} A^T \lambda - b^T \lambda \\ \text{subject to} & \lambda \geq 0 \end{array}$$

- from Slater's condition: $p^\star = d^\star$ if $A\tilde{x} < b$ for some $\tilde{x}$
- $p^\star = d^\star$ always

Mind the Duality Gap

Theory: Zero duality gap is a certificate of optimality
Thought Experiment:

- Todd gives Munir a primal solution x and claims it is optimal.
- Munir trusts Todd but everyone can make an honest mistake, even Todd.
- How can Munir check Todd's claim?

Solution:

- Todd can provide not only an x but also (λ, ν).
- Munir plugs x into $\psi_P(x)$ and (λ, ν) into $\psi_D(\lambda, \nu)$
- Does $\psi_P(x) = \psi_D(\lambda, \nu)$?

Mind the Duality Gap

Practical Consequence: Debugging your code / checking for correctness

Scenario 1:

- Your iterative algorithm for solving a problem that admits strong duality has been running for 1000 hours. The duality gap hasn't changed since the first minute of running.
- You probably have a bug in your code.
- You want to see the duality gap tending towards zero.

Mind the Duality Gap

Practical Consequence: Debugging your code / checking for correctness

Scenario 2:

- Someone else's iterative algorithm for solving a problem that admits strong duality has been running for 1000 hours. The duality gap hasn't changed since the first minute of running.
- They probably have a bug in their code.
- You want to see the duality gap tending towards zero.

Mind the Duality Gap

Practical Consequence: Debugging your code / checking for correctness

Scenario 3:

- Your collaborator / advisor doesn't trust the results from your estimator. They tell you they suspect your code is buggy.
- You show that the duality gap on some benchmark problems goes to machine precision, verifying that your code is correct.
- This leads to you and your collaborator / advisor to determine a fundamental flaw in your original estimator which inspires a modification that addresses a non-trivial open problem.
- You publish your paper in JASA T&M

Duality for Unconstrained Problems

$$\text{minimize } f_0(Ax + b)$$

- dual function is constant:
  $\psi_D = \inf_x \mathcal{L}(x) = \inf_x f_0(Ax + b) = p^\star$
- we have strong duality, but dual isn't helpful

Key Idea: Introduce new variables and equality constraints

Equivalent equality constrained problem

$$\begin{aligned} &\underset{x,y}{\text{minimize}} && f_0(y) \\ &\text{subject to} && Ax + b - y = 0 \end{aligned}$$

Duality for Unconstrained Problems

Equivalent equality constrained problem

$$\begin{aligned} &\underset{x,y}{\text{minimize}} && f_0(y) \\ &\text{subject to} && Ax + b - y = 0 \end{aligned}$$

Dual function

$$\begin{aligned} \psi_D(\nu) &= \inf_{x,y} \left(f_0(y) - \nu^T y + \nu^T A x + b^T \nu \right) \\ &= \begin{cases} -f_0^\star(\nu) + b^T \nu & A^T \nu = 0 \\ -\infty & \text{o.w.} \end{cases} \end{aligned}$$

Dual problem

$$\begin{aligned} &\underset{x,y}{\text{minimize}} && b^T \nu - f_0^\star(\nu) \\ &\text{subject to} && A^T \nu = 0 \end{aligned}$$

Duality for least squares regression

$$\underset{b}{\text{minimize}} \ \|y - Xb\|_2^2$$

$$\underset{b,z}{\text{minimize}} \ \|z\|_2^2$$

$$\text{subject to } y - Xb = z$$

Fenchel conjugate

$$f^\star(v) = \sup_{u \in \text{dom} f} v^T u - f(u)$$

Fenchel conjugate of quadratic

$$f_0(u) = u^T u \qquad f_0^\star(v) = \frac{1}{4} v^T v$$

Dual Problem

$$\underset{\nu}{\text{maximize}} \ y^T \nu - \frac{1}{4}\|\nu\|_2^2$$

$$\text{subject to } X^T \nu = 0$$

Complementary Slackness

Assume strong duality holds, $x^\star$ is primal optimal, $(\lambda^\star, \nu^\star)$ is dual optimal.

$$\begin{aligned} f_0(x^\star) = \psi_D(\lambda^\star, \nu^\star) &= \inf_x \left(f_0(x) + \sum_{i=1}^m \lambda_i^\star f_i(x) + \sum_{i=1}^p \nu_i^\star h_i(x) \right) \\ &\leq f_0(x^\star) + \sum_{i=1}^m \lambda_i^\star f_i(x^\star) + \sum_{i=1}^p \nu_i^\star h_i(x^\star) \\ &\leq f_0(x^\star) \end{aligned}$$

- $x^\star$ minimizes $\mathcal{L}(x, \lambda^\star, \nu^\star)$
- $\lambda_i^\star f_i(x^\star) = 0$ for $i = 1, \ldots, m$ (complementary slackness condition)

$$\lambda_i^\star > 0 \implies f_i(x^\star) = 0, \quad f_i(x^\star) < 0 \implies \lambda_i^\star = 0$$

Karush-Kuhn-Tucker (KKT) conditions

the following four conditions are called KKT conditions (for a problem with differentiable f_i, h_i):

- **primal feasibility:**
  $f_i(x) \leq 0, i = 1, \ldots, m, h_i(x) = 0, i = 1, \ldots, p$
- **dual feasibility:** $\lambda \geq 0$
- **complementary slackness:** $\lambda_i f_i(x) = 0, i = 1, \ldots, m$
- **stationarity:** gradient of Lagrangian vanishes with respect to x:

$$\nabla_x \mathcal{L}(x, \lambda, \nu) = \nabla f_0(x) + \sum_{i=1}^{m} \lambda_i \nabla f_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x)$$

- if strong duality holds and x, λ, ν are optimal, then they must satisfy the KKT conditions

KKT conditions for convex problems

if $\tilde{x}, \tilde{\lambda}, \tilde{\nu}$ satisfy KKT for a convex problem, then they are optimal:

- from complementary slackness: $f_0(\tilde{x}) = \mathcal{L}(\tilde{x}, \tilde{\lambda}, \tilde{\nu})$
- from stationarity (and convexity): $\psi_D(\tilde{\lambda}, \tilde{\nu}) = \mathcal{L}(\tilde{x}, \tilde{\lambda}, \tilde{\nu})$ hence, $f_0(\tilde{x}) = \psi_D(\tilde{\lambda}, \tilde{\nu})$

if Slater's condition is satisfied: x is optimal if and only if there exist λ, ν that satisfy KKT conditions

- recall that Slater implies strong duality, and dual optimum is attained
- generalizes optimality condition $\nabla f_0(x) = 0$ for unconstrained problem

KKT Conditions: Nonnegative Least Squares

$$\min_{b \geq 0} f(b) := \frac{1}{2}\|y - Xb\|_2^2$$

Lagrangian:

$$\mathcal{L}(b, \lambda) = \frac{1}{2}\|y - Xb\|_2^2 - \lambda^T b$$

- **primal feasibilty:**
- **dual feasibility:** $\lambda \geq 0$
- **complementary slackness:**
- **stationarity:**

KKT Conditions: Nonnegative Least Squares

$$\nabla f(b) = X^T(Xb - y)$$

$b^\star$ is a global solution iff

$$\begin{aligned} b^\star &\geq 0 \\ \nabla f(b^\star) &\geq 0 \\ [\nabla f(b^\star)]_j b_j^\star &= 0. \end{aligned}$$

From KKT conditions to a stopping rule

KKT conditions:

$$\begin{aligned} b^\star &\geq 0 \\ \nabla f(b^\star) &\geq 0 \\ [\nabla f(b^\star)]_j b_j^\star &= 0. \end{aligned}$$

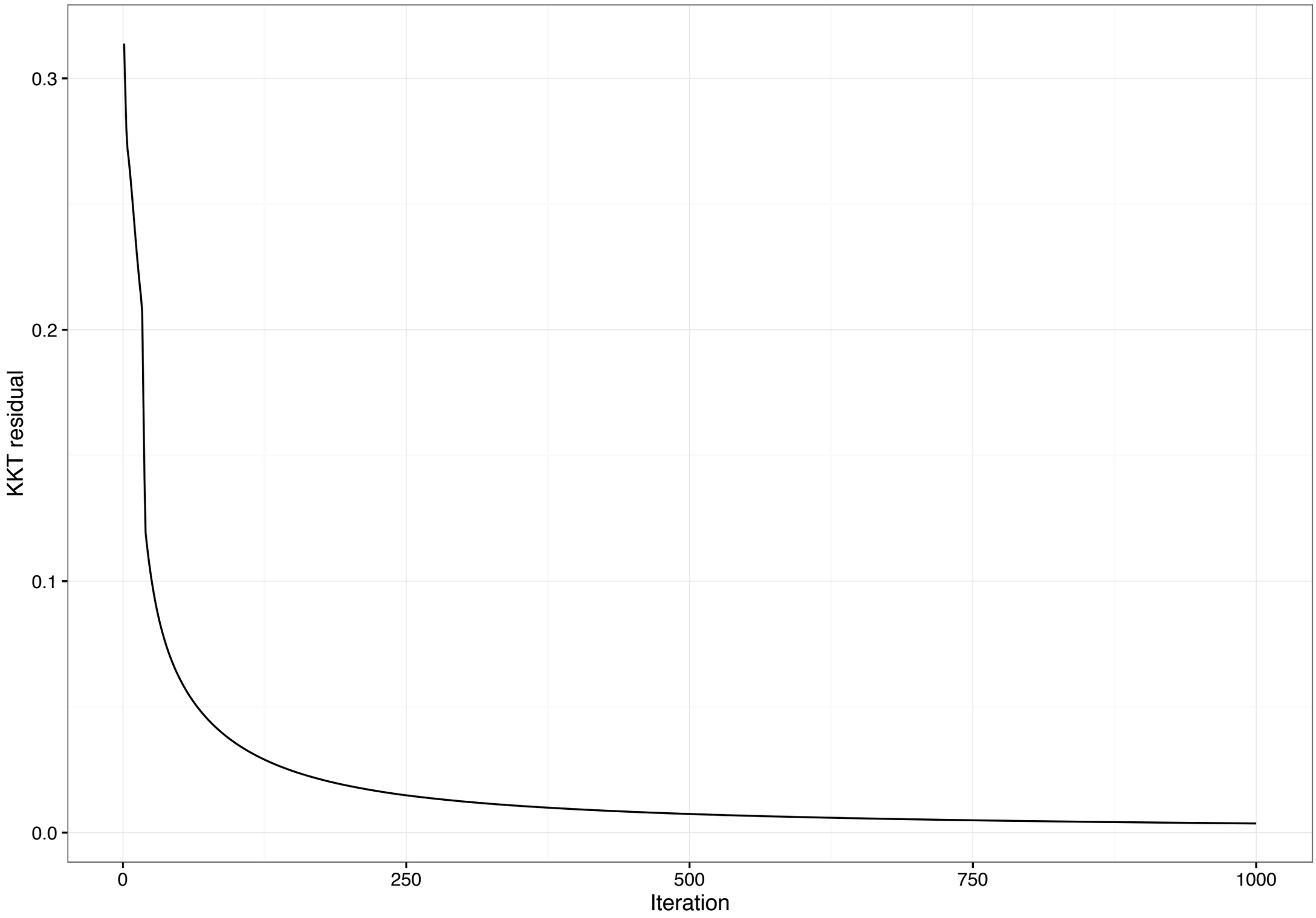
If $b_n \to b^\star$, then

$$\min(b_{nj}, [\nabla f(b_n)]_j) \to 0$$

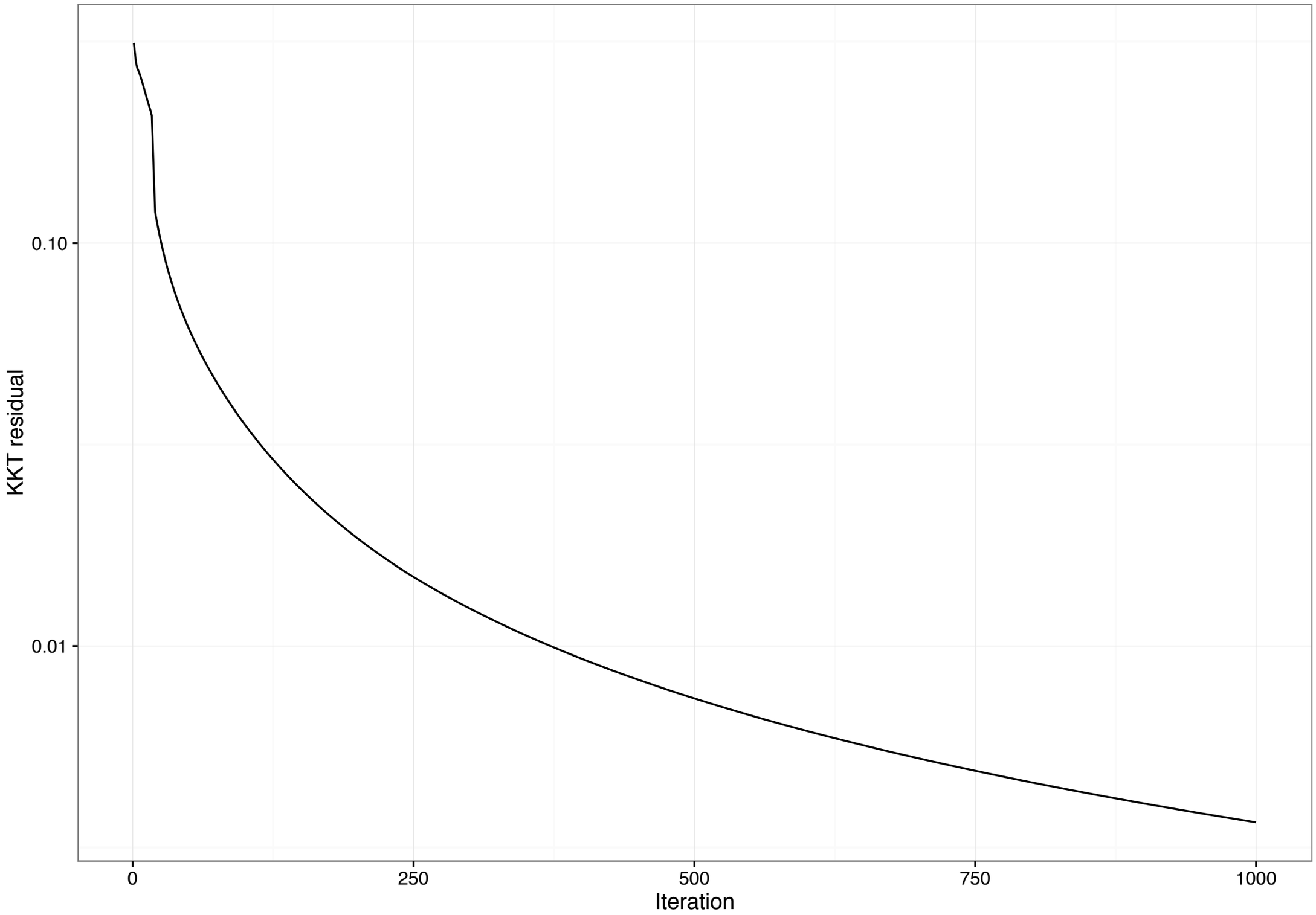
KKT residual:

$$\max_{j=1,\ldots,p} [\min(b_{nj}, [\nabla f(b_n)]_j)] \to 0$$

Track progress with KKT residuals



Track progress with KKT residuals

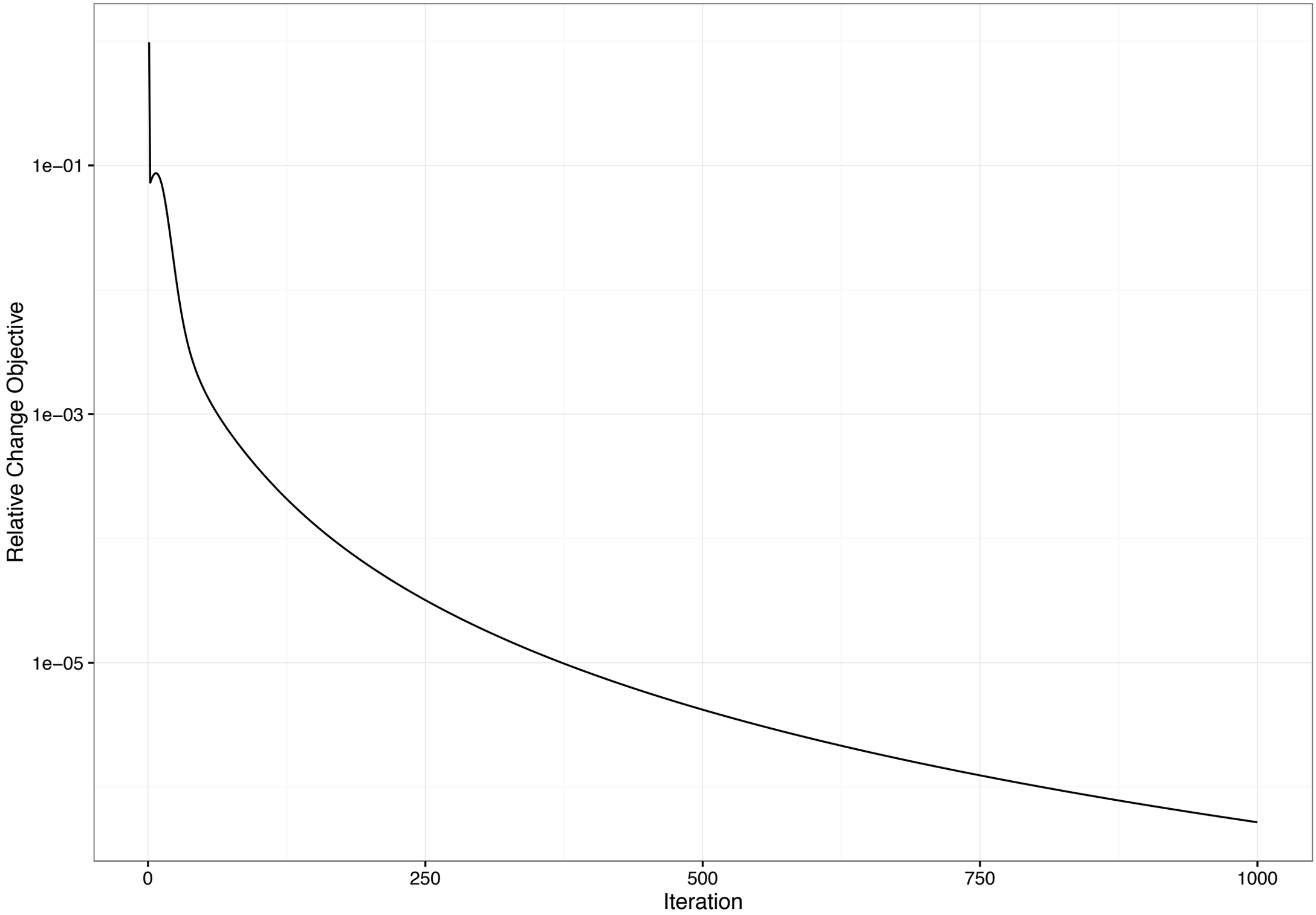


Track progress with relative change in objective

Stop when

$$\frac{f(b) - f(b^+)}{1 + |f(b)|} \leq \text{tolerance}$$

Track progress with relative change in objective

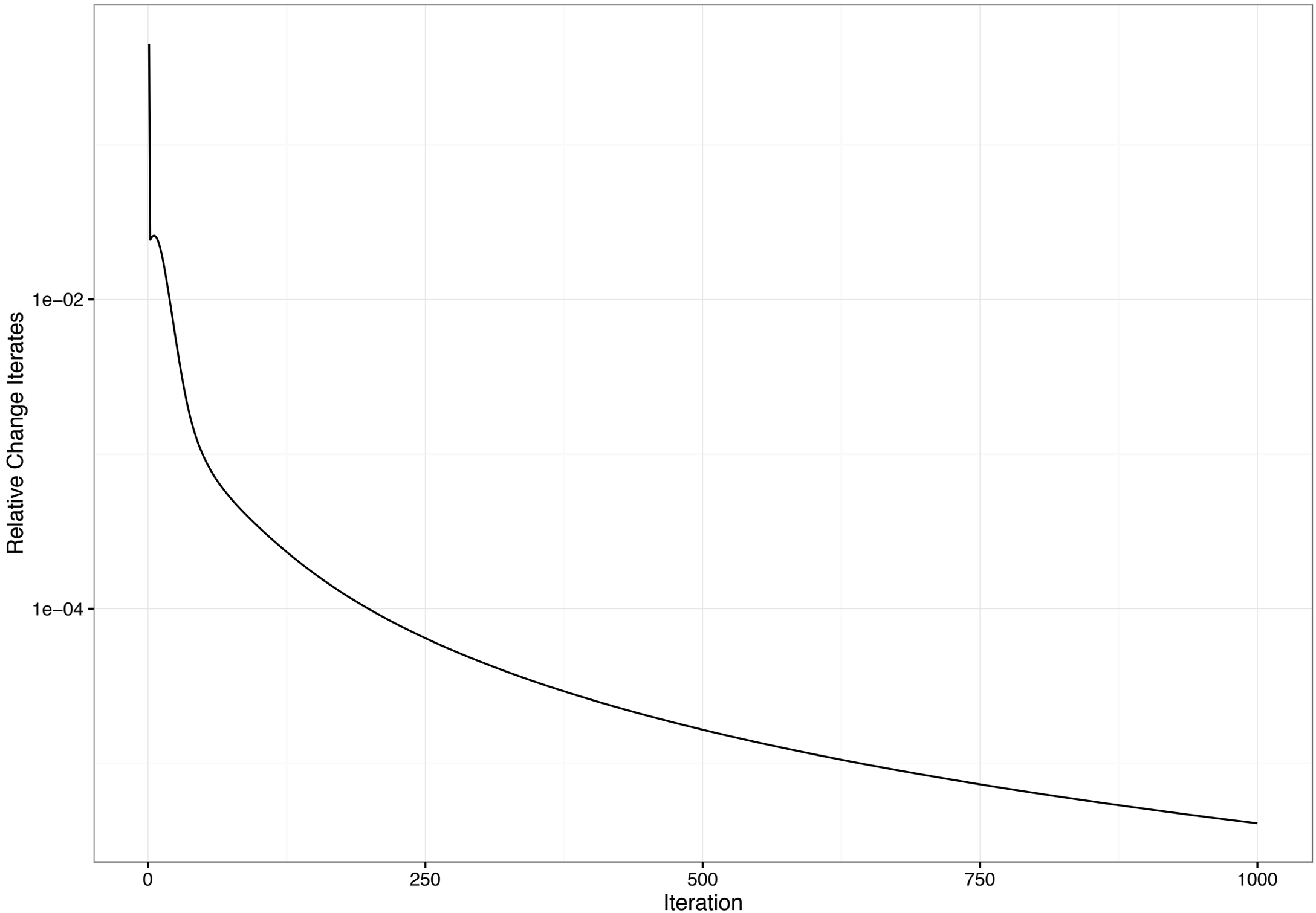


Track progress with relative change in iterates

Stop when

$$\frac{\|b - b^+\|}{1 + \|b\|} \leq \text{tolerance}$$

Track progress with relative change in iterates



Least Absolute Shrinkage and Selection Operator (LASSO)

$$\text{minimize } \|y - Xb\|_2^2 + \gamma \|b\|_1$$

KKT conditions for Lasso

$$\min_{b^+,b^- \geq 0} f(b) := \frac{1}{2}\|y - Xb^+ + Xb^-\|_2^2 + \gamma\langle 1, b^+\rangle + \gamma\langle 1, b^-\rangle$$

Lagrangian:

$$\mathcal{L}(b,\lambda) = \frac{1}{2}\|y - Xb^+ + Xb^-\|_2^2 + \gamma\langle 1, b^+\rangle + \gamma\langle 1, b^-\rangle - \langle \lambda^+, b^+\rangle - \langle \lambda^-, b^-\rangle$$

- **primal feasibilty:** $b^+, b^- \geq 0$
- **dual feasibility:** $\lambda^+, \lambda^- \geq 0$
- **complementary slackness:** $\lambda_j^+ b_j^+ = \lambda_j^- b_j^- = 0$
- **stationarity:**

$$\nabla f(b) + \gamma 1 - \lambda^+ = 0$$
$$-\nabla f(b) + \gamma 1 - \lambda^- = 0$$

KKT conditions for Lasso

- $\|\nabla f(b)\|_\infty \leq \gamma$
- if $b_j > 0$ then $[\nabla f(b)]_j = -\gamma$
- if $b_j < 0$ then $[\nabla f(b)]_j = \gamma$

Q: For what value of γ is $b = 0$ the solution?

Checking convergence:

- Simple / insufficient: $[\|\nabla f(b_n)\|_\infty - \gamma]_+ \to 0$
- More complicated:

$$\max_j \tau(b, j) \to 0$$

where

$$\tau(b,j) = \begin{cases} |[\nabla f(b)]_j + \gamma| & b_j > 0 \\ |[\nabla f(b)]_j - \gamma| & b_j < 0 \\ [|[\nabla f(b)]_j| - \gamma]_+ & b_j = 0 \end{cases}$$

General Principles

- Use KKT conditions (and duality gap) to check your code on small problems for correctness
- In released code, use more lenient stopping criteria (relative change in objective).

Some History on Karush-Kuhn-Tucker

- 1939: William Karush's master's thesis
- 1951: Harold Kuhn and Albert Tucker paper
- 1975: Kuhn sets the record straight by at AMS Symposium on "Nonlinear Programming - A Historical View"

Karush replying to correspondence initiated by Kuhn:

"The thought of publication never occurred to me at the time I wrote the master's thesis. I was a struggling graduate student trying to meet the requirements for going on to my Ph.D. and Graves never brought up the question of publication. I imagine nobody at that time anticipated the future interest in the problem."

What's Duality Good For?

Certify that your algorithm is correct

- duality gap and KKT conditions

→ **Broaden your algorithm design menu**

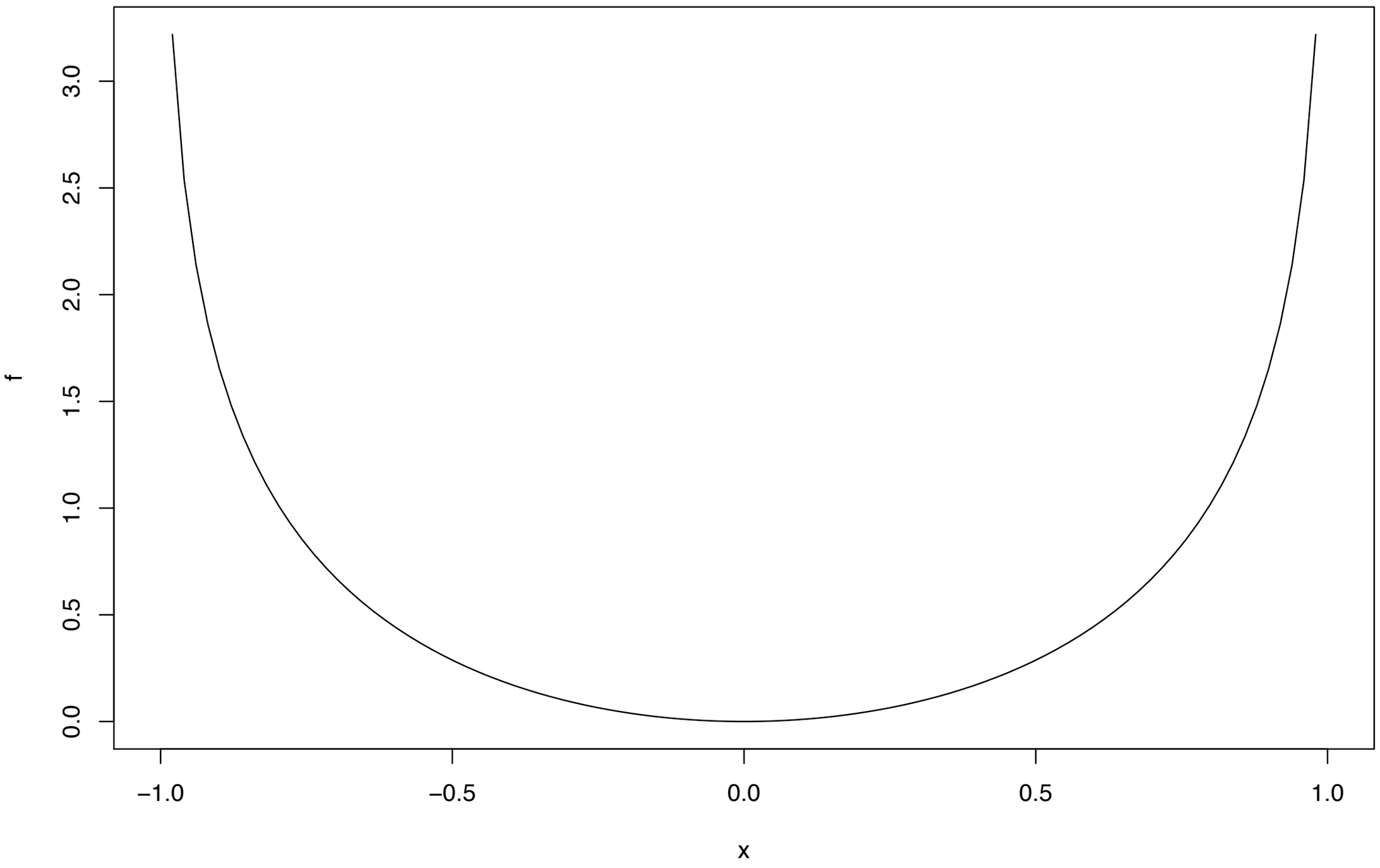
- You could solve the primal problem, but solving the dual problem takes less time to develop code, has better numerical properties, etc.

Closed Convex Functions

Definition: A function f is closed if its epigraph is a closed set

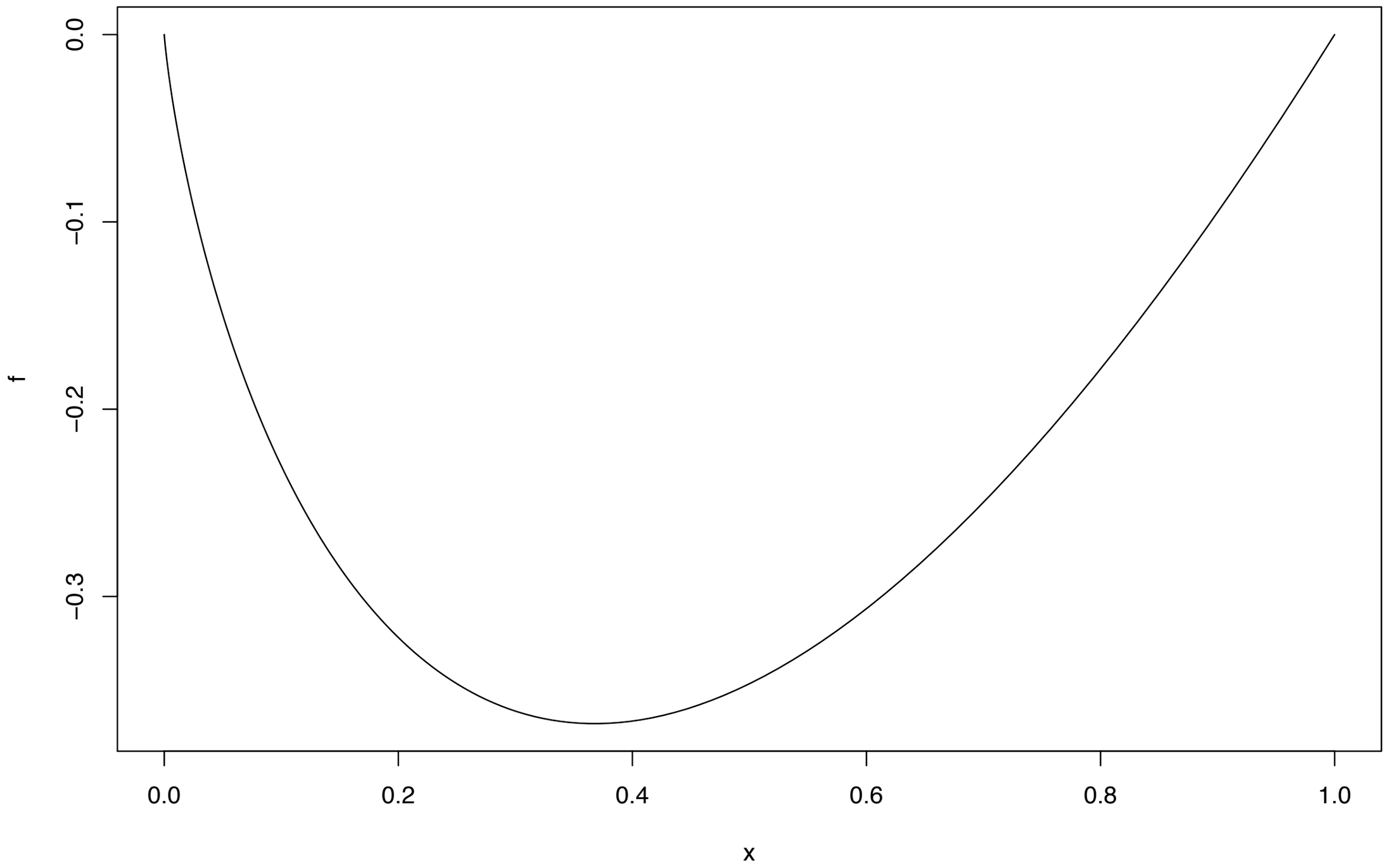
Examples of Closed Convex Functions

$$f(x) = -\log(1 - x^2) \text{ with } \operatorname{dom} f = \{x : |x| < 1\}$$



Examples of Closed Convex Functions

$$f(x) = x \log(x) \text{ with } \operatorname{dom} f = \mathbb{R}_+ \text{ and } f(0) = 0$$



More on Conjugate Functions

Fenchel conjugate of a function f is

$$f^\star(y) = \sup_{x \in \mathbf{dom}\, f} (y^T x - f(x))$$

- $f^\star$ is closed and convex even if f is not
- Fenchel's inequality

$$f(x) + f^\star(y) \geq x^T y, \quad \forall x, y$$

The Second Conjugate

$$f^{\star\star}(x) = \sup_{y \in \mathrm{dom}\, f^\star} (x^T y - f^\star(y))$$

- $f^{\star\star}$ is closed and convex - From Fenchel inequality

$$f^{\star\star}(x) \leq f(x) \quad \forall x$$

- if f is closed and convex, then $f^{\star\star} = f$

Conjugates and Subgradients

if f is closed and convex, then

$$y \in \partial f(x) \iff x^T y = f(x) + f^\star(y) \iff x \in \partial f^\star(y)$$

proof: if $y \in \partial f(x)$, then for all u

$$f(u) \geq f(x) + y^T(u - x)$$
$$y^T x - f(x) \geq y^T u - f(u)$$

Therefore, $f^\star(y) = y^T x - f(x)$.

Conjugates and Subgradients

if f is closed and convex, then

$$y \in \partial f(x) \iff x^T y = f(x) + f^\star(y) \iff x \in \partial f^\star(y)$$

proof: if $x^T y = f(x) + f^\star(y)$, then $f^\star(y) = x^T y - f(x)$

$$\implies 0 \in y - \partial f(x)$$
$$\implies y \in \partial f(x)$$

Conjugates and Subgradients

if f is closed and convex, then

$$y \in \partial f(x) \iff x^T y = f(x) + f^\star(y) \iff x \in \partial f^\star(y)$$

proof: if $x \in \partial f^\star(y)$, then for all v

$$f(v) \geq f^\star(y) + x^T(v - y)$$
$$x^T y - f^\star(y) \geq x^T v - f^\star(v)$$

Therefore, $f^{\star\star}(x) = x^T y - f^\star(y)$. Since $f^{\star\star} = f$

$$f(x) + f^\star(y) = x^T y$$

Conjugates and Subgradients

if f is closed and convex, then

$$y \in \partial f(x) \iff x^T y = f(x) + f^\star(y) \iff x \in \partial f^\star(y)$$

proof: if $x^T y = f(x) + f^\star(y)$, then $f^{\star\star}(x) = x^T y - f^\star(y)$, since $f^{\star\star} = f$.

$$\implies 0 \in x - \partial f^\star(y)$$

$$\implies x \in \partial f^\star(y)$$

Dual Norm

dual norm of a norm $\|\cdot\|$ is

$$\|y\|_* = \sup_{\|x\| \leq 1} y^T x$$

$\|y\|_*$ is the support function of the unit ball for $\|\cdot\|$

- common pairs of dual vector norms:

$$\|x\|_2, \|y\|_2, \quad \|x\|_1, \|y\|_\infty, \quad \sqrt{x^T Q x}, \sqrt{y^T Q^{-1} y}\,(Q \in S_{++})$$

- common pairs of dual matrix norms

$$\|X\|_{\mathrm{F}}, \|Y\|_{\mathrm{F}}, \quad \|X\|_{\mathrm{op}} = \sigma_{\max}(X) = \|X\|_2, \|Y\|_* = \sum_i \sigma_i(Y)$$

Conjugate of Norm

conjugate of $f = \|x\|$ is the indicator function of the dual unit norm ball

$$f^\star(y) = \sup_x \left(y^T x - \|x\|\right) = \begin{cases} 0 & \|y\|_* \leq 1 \\ +\infty & \text{o.w.} \end{cases}$$

proof:

- if $\|y\|_* \leq 1$, then (by definition of dual norm) $\forall x$

$$\frac{y^T x}{\|x\|} \leq 1$$

$$y^T x \leq \|x\|$$

  and equality holds when $x = 0$; therefore $\sup_x(y^T x - \|x\|) = 0$
- if $\|y\|_* > 1$ then there exists an x with $\|x\| \leq 1, y^T x > 1$; then

$$f^\star(y) \geq y^T(tx) - \|tx\| = t(y^T x - \|x\|) \to \infty \text{ as } t \to \infty$$

Moreau Decomposition

$$x = \text{prox}_h(x) + \text{prox}_{h^\star}(x) \quad \forall x$$

proof:

$$\begin{aligned} u = \text{prox}_h(x) &\iff x - u \in \partial h(x) \\ &\iff u \in \partial h^\star(x - u) \\ &\iff x - u = \text{prox}_{h^\star}(x) \end{aligned}$$

- Generalizes decomposition by orthogonal projection onto subspaces:

  $$x = P_L(x) + P_{L^\perp}(x)$$

  if L is a subspace, $L^\perp$ its orthogonal complement.

(this is the Moreau decomposition with $h = \delta_L, h^\star = \delta_{L^\perp}$)

Basic rules for Proximal Maps

separable sum: $h(x_1, x_2) = h_1(x_1) + h_2(x_2)$

$$\mathrm{prox}_h(x_1, x_2) = (\mathrm{prox}_{h_1}(x_1), \mathrm{prox}_{h_2}(x_2))$$

scaling and translation of argument: $h(x) = f(\lambda x + a)$ with $\lambda \neq 0$

$$\mathrm{prox}_h(x) = \frac{1}{\lambda}(\mathrm{prox}_{\lambda^2 f}(\lambda x + a) - a)$$

conjugate: for $t > 0$

$$\mathrm{prox}_{th^\star}(x) = x - t\,\mathrm{prox}_{h/t}(x/t)$$

for $t = 1$ this is the Moreau decomposition

Support Function

conjugate of support function of closed convex set is indicator function

$$h(x) = S_C(x) = \sup_{y \in C} x^T y, \quad h^\star(y) = \delta_C(y)$$

prox-operator of support function:

$$\begin{aligned} \mathrm{prox}_{th}(x) &= x - t\,\mathrm{prox}_{h^\star/t}(x/t) \\ &= x - tP_C(x/t) \end{aligned}$$

Norms

conjugate of norm is the indicator function of the dual norm ball:

$$h(x) = \|x\|, \quad h^\star(y) = \delta_B(y) \quad (B = \{y : \|y\|_* \leq 1\})$$

prox-operator of norm

$$\begin{aligned}\text{prox}_{th}(x) &= x - t\,\text{prox}_{h^\star/t}(x/t) \\ &= x - tP_B(x/t)\end{aligned}$$

useful for computing $\text{prox}_{t\|\cdot\|}$ when P_B is inexpensive

Soft-Thresholding Operator

- $h(x) = \|x\|_1, B = \{y : \|y\|_\infty \leq 1\}$

Duality and Conjugates

primal problem ($A \in \mathbb{R}^{m \times n}$, f and g convex)

$$\text{minimize } f(x) + g(Ax)$$

Lagrangian (after introducing new variable $y = Ax$)

$$f(x) + g(y) + \langle z, Ax - y \rangle$$

Dual function

$$\inf_x \ (f(x)) + \langle z, Ax \rangle) + \inf_y \ (g(y) - \langle z, y \rangle) = -f^\star(-A^T z) - g^\star(z)$$

Dual problem

$$\text{maximize } \ -f^\star(-A^T z) - g^\star(z)$$

Example: Equality Constraints

g is indicator for $\{b\}$

Primal:

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } Ax = b \end{aligned}$$

$$g^\star(z) = \sup_{y \in \{b\}} \langle y, z \rangle = \langle b, z \rangle$$

Dual:

$$\text{maximize } -f^\star(-A^T z) - \langle b, z \rangle$$

Example: Linear inequality constraints

g is indicator for $\{y : y \leq b\}$

Primal:

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } Ax \leq b \end{aligned}$$

$$\begin{aligned} g^\star(z) &= \sup_{y \leq b} \langle y, z \rangle \\ &= \sup_{y-b \leq 0} \langle y - b, z \rangle + \langle b, z \rangle \\ &= \langle b, z \rangle + \delta_C(z), \end{aligned}$$

where $C = \{z : z \geq 0\}$

Dual:

$$\begin{aligned} &\text{maximize } -f^\star(-A^T z) - \langle b, z \rangle \\ &\text{subject to } z \geq 0 \end{aligned}$$

Example: Norm regularization

$$g(y) = \|y - b\|$$

Primal:

$$\text{minimize } f(x) + \|Ax - b\|$$

$$g^\star(z) = \langle b, z\rangle + \delta_C(z),$$

where $C = \{z : \|z\|_\dagger \leq 1\}$

Dual:

$$\text{maximize } -f^\star(-A^T z) - \langle b, z\rangle$$

$$\text{subject to } \|z\|_\dagger \leq 1$$

Dual methods

Apply first-order method to the dual problem

$$\text{maximize} \;\; -f^\star(-A^T z) - g^\star(z)$$

Why might the dual be easier for a first-order method?

- Dual problem is unconstrained or has simple constraints
- Dual objective is differentiable or has a simple non-differentiable term
- Decomposition: exploit separable structure

(Sub-)gradients of conjugate function

Assume $f : \mathbb{R}^n \to \mathbb{R}$ is closed and convex with conjugate

$$f^\star(y) = \sup_x \left(\langle y, x\rangle - f(x)\right)$$

subgradient

- $f^\star$ is subdifferentiable on (at least) **int dom** $f^\star$
- maximizers in the definition of $f^\star(y)$ are subgradients at y

$$y \in \partial f(x) \iff \langle y, x\rangle - f(x) = f^\star(y) \iff x \in \partial f^\star(y)$$

gradient: for strictly convex f, maximizer in definition is unique if it exists

$$\nabla f^\star(y) = \arg\max_x \left(\langle y, x\rangle - f(x)\right)$$

if maximum is attained

Conjugate of strongly convex function

Assume f is closed and **strongly** convex, with parameter $\mu > 0$

- $f^\star$ is defined for all y, namely **dom** $f^\star = \mathbb{R}^n$
- $f^\star$ is differentiable everywhere, with gradient

$$\nabla f^\star(y) = \arg\max_x \; (\langle y, x\rangle - f(x))$$

- $\nabla f^\star$ is Lipschitz continuous with constant $1/\mu$

$$\|\nabla f^\star(y) - \nabla f^\star(\tilde{y})\|_2 \leq \frac{1}{\mu}\|y - \tilde{y}\|_2 \quad \forall y, \tilde{y}$$

Composite structure in the dual

Primal:

$$\text{minimize } f(x) + g(Ax)$$

Dual:

$$\text{maximize } -f^\star(-A^T z) - g^\star(z)$$

dual has the right structure for the proximal gradient method if

- prox-operator of g (or $g^\star$) is cheap (closed form or simple algorithm)
- f is strongly convex because then $f^\star(-A^T z)$ has Lipschitz continuous gradient ($L = \|A\|_2^2/\mu$):

$$\|A\nabla f^\star(-A^T u) - A\nabla f^\star(-A^T v)\|_2 \leq \frac{\|A\|_2^2}{\mu}\|u - v\|_2$$

Dual Proximal Gradient Method

$$z^+ = \mathrm{prox}_{tg^\star}\left(z + tA\nabla f^\star(-A^T z)\right)$$

equivalent expression in terms of f:

$$\hat{x} = \arg\min_x \ (f(x) + \langle z, Ax\rangle)$$
$$z^+ = \mathrm{prox}_{tg^\star}\left(z + tA\hat{x}\right)$$

- if f is separable, calculation of $\hat{x}$ decomposes into independent problems
- step size t constant or from backtracking line search
- if $g^\star$ is separable, calculation of z^+ decomposes into independent problems
- can use accelerated first order methods (FISTA, BB)

Alternating minimization interpretation

Recall conjugate rule for prox-operators: for $t > 0$

$$\mathrm{prox}_{tg^\star}(x) = x - t\mathrm{prox}_{g/t}(x/t)$$

Alternative expression for z-update

$$z^+ = z + t(A\hat{x} - \hat{y})$$

where

$$\begin{aligned}
\hat{x} &= \arg\min_x \ (f(x) + \langle z, Ax\rangle) \\
\hat{y} &= \mathrm{prox}_{t^{-1}g}\,(z/t + A\hat{x}) \\
&= \arg\min_y \ \left(g(y) + \langle z, A\hat{x} - y\rangle + \frac{t}{2}\|A\hat{x} - y\|_2^2\right)
\end{aligned}$$

in each iteration, an alternating minimization of:

- Lagrangian $f(x) + g(y) + \langle z, Ax - y\rangle$ over x
- augmented Lagrangian $f(x) + g(y) + \langle z, Ax - y\rangle + \frac{t}{2}\|Ax - y\|_2^2$

Minimization over intersection of convex sets

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } x \in C_1 \cap \cdots \cap C_m \end{aligned}$$

- f strongly convex
- sets C_i are closed, convex, and easy to project onto

$$g(y_1, \ldots, y_m) = \delta_{C_1}(y_1) + \cdots + \delta_{C_m}(y_m)$$

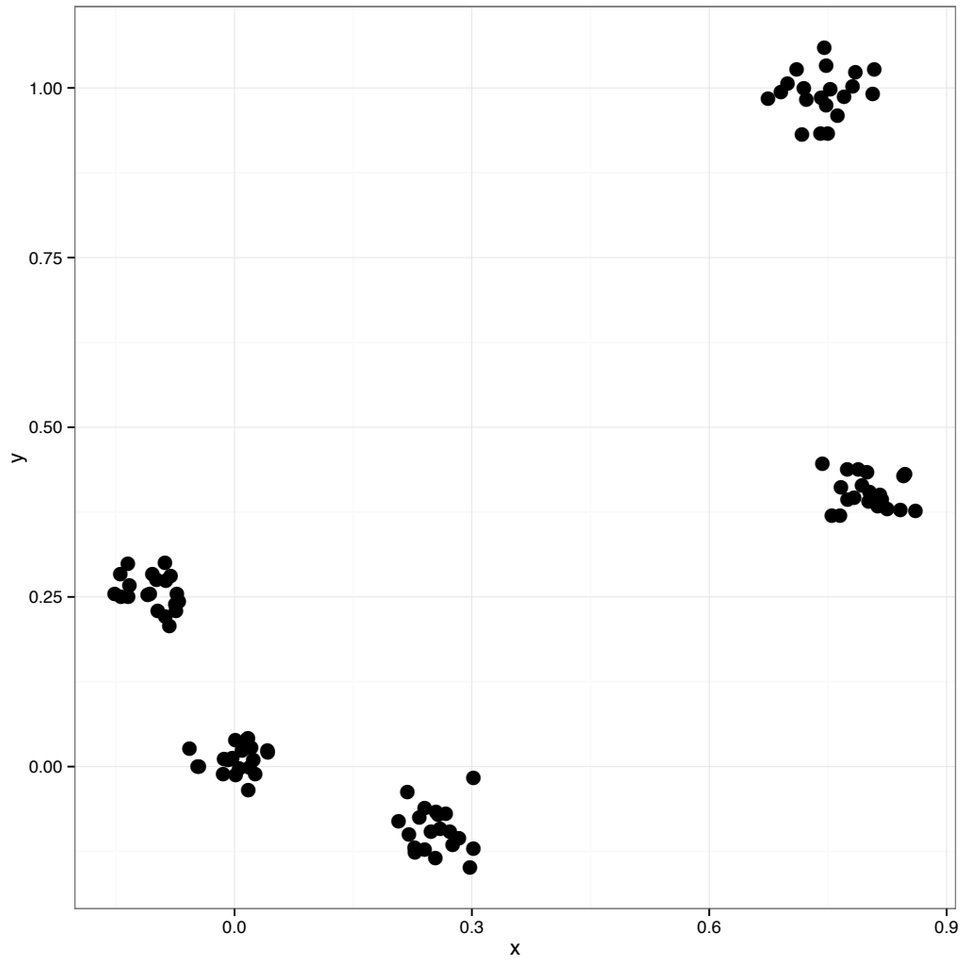
$$A = \begin{pmatrix} I & \cdots & I \end{pmatrix}^T$$

dual proximal gradient update

$$\hat{x} = \arg\min_x \; f(x) + \langle x, \sum_{i=1}^m z_i \rangle$$

$$z_i^+ = z_i + t\hat{x} - tP_{C_i}(z_i/t + \hat{x}), \quad i = 1, \ldots, m$$

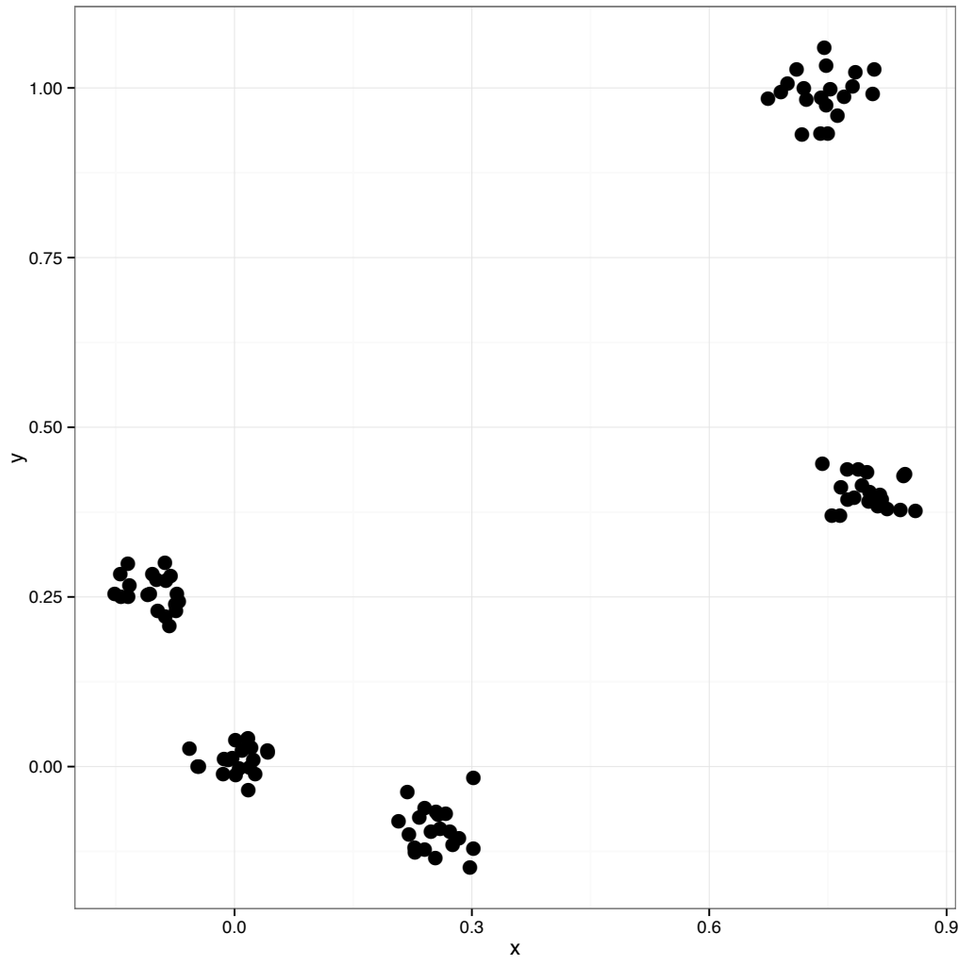
The Clustering Problem



Task:

- Given p points in q dimensions
- $\mathbf{X} \in \mathbb{R}^{q \times p}$
- group similar points together.

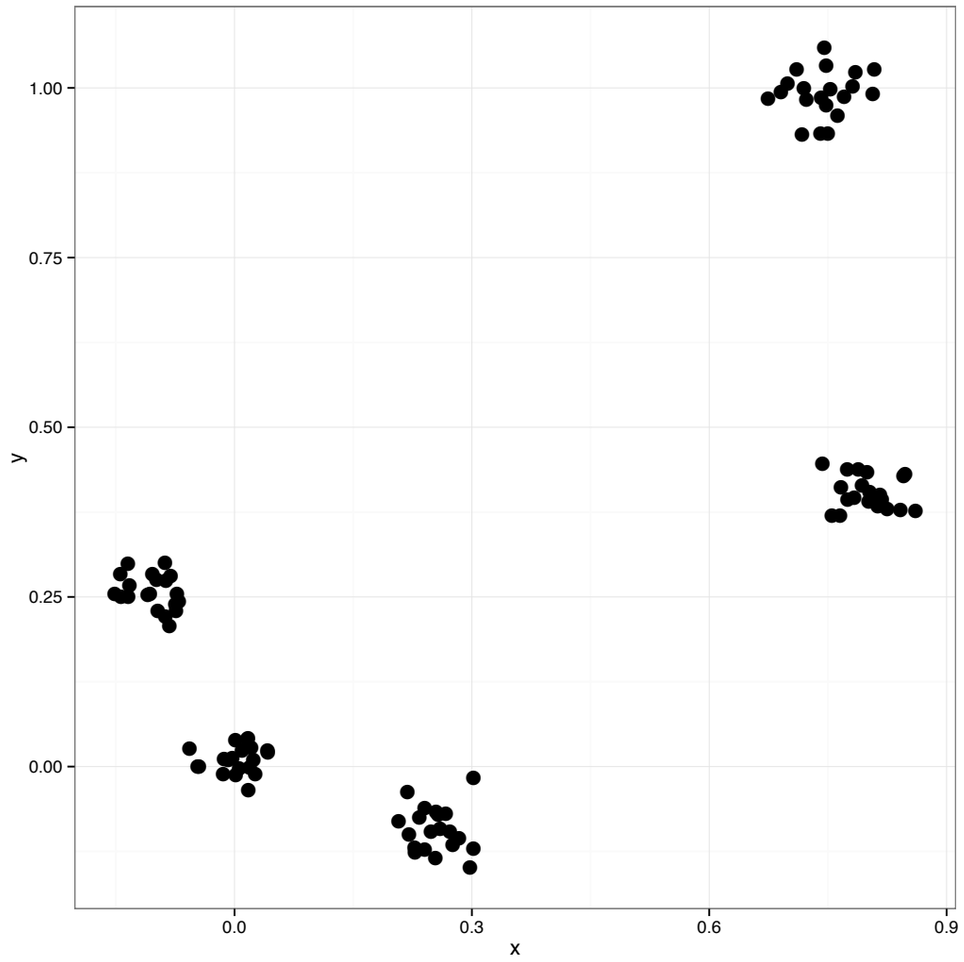
The Clustering Problem



Many approaches:

- k-means, mixture models
- Hierarchical clustering
- Spectral clustering, ...

The Clustering Problem



Computational Issues

- Nonconvex formulations
- Local minimizers
- Instability (initializations, tuning parameters, or data)

Convex Clustering

- Pelckmans et al. 2005, Lindsten et al. 2011, Hocking et al. 2011

$$\underset{\mathbf{u}}{\text{minimize}} \frac{1}{2} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{u}_i\|_2^2$$

- Assign a centroid $\mathbf{u}_i$ to each data point $\mathbf{x}_i$.

Convex Clustering

- Pelckmans et al. 2005, Lindsten et al. 2011, Hocking et al. 2011

$$\underset{\mathbf{u}}{\text{minimize}} \; \frac{1}{2} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{u}_i\|_2^2$$

- Assign a centroid $\mathbf{u}_i$ to each data point $\mathbf{x}_i$.

Too many degrees of freedom!

Convex Clustering

- Pelckmans et al. 2005, Lindsten et al. 2011, Hocking et al. 2011

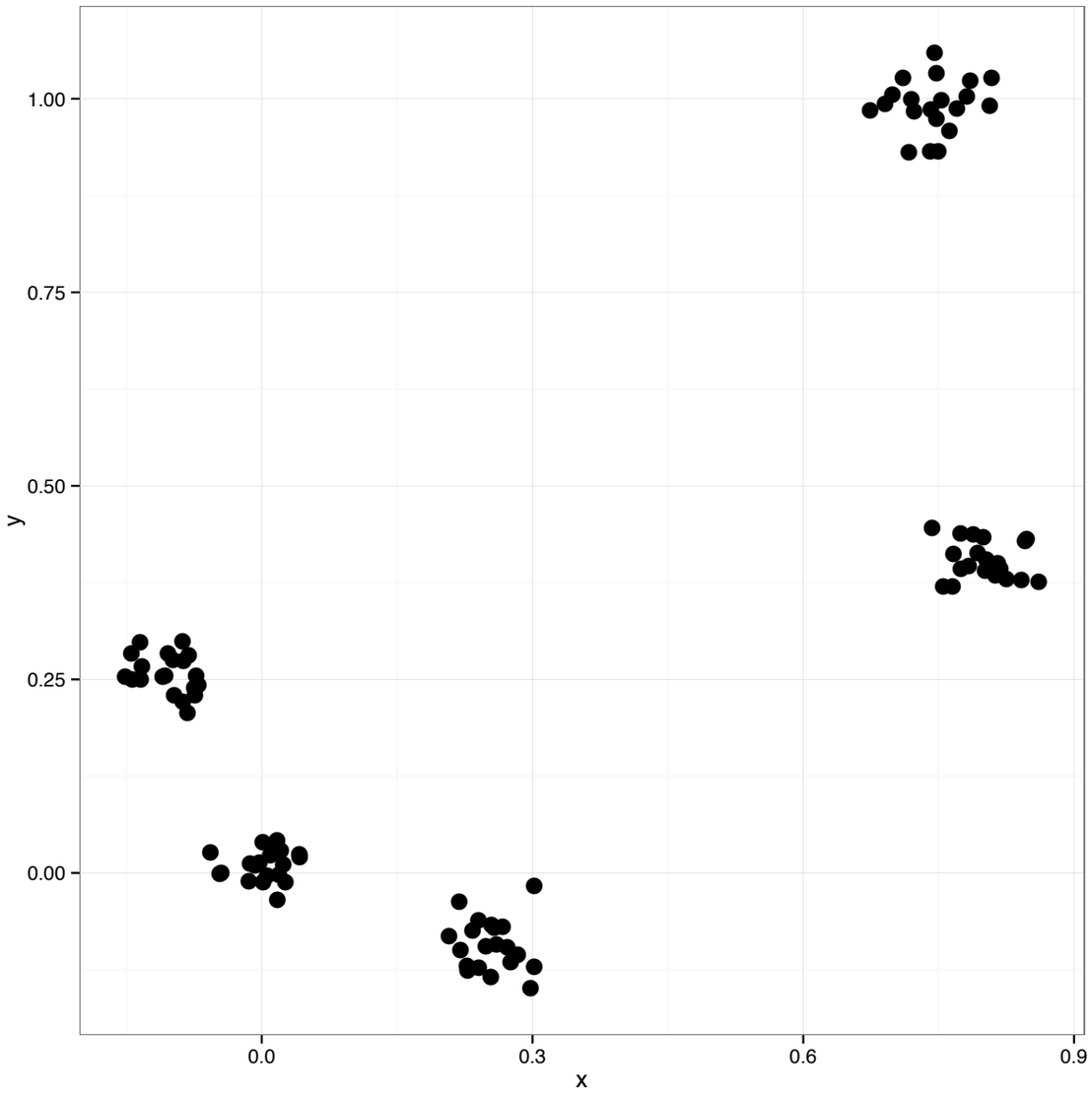
$$\underset{\mathbf{u}}{\text{minimize}} \; \frac{1}{2} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij} \|\mathbf{u}_i - \mathbf{u}_j\|_2$$

- Assign a centroid $\mathbf{u}_i$ to each data point $\mathbf{x}_i$.
- Convex Fusion Penalty
  - shrinks cluster centroids together
  - sparsity in pairwise differences of centroids

$$\mathbf{u}_i - \mathbf{u}_j = \mathbf{0} \iff \mathbf{x}_i \text{ and } \mathbf{x}_j \text{ belong to the same cluster}$$

- γ : tunes overall amount of regularization
- w_{ij} : fine tunes pairwise shrinkage
- Generalizes fused lasso

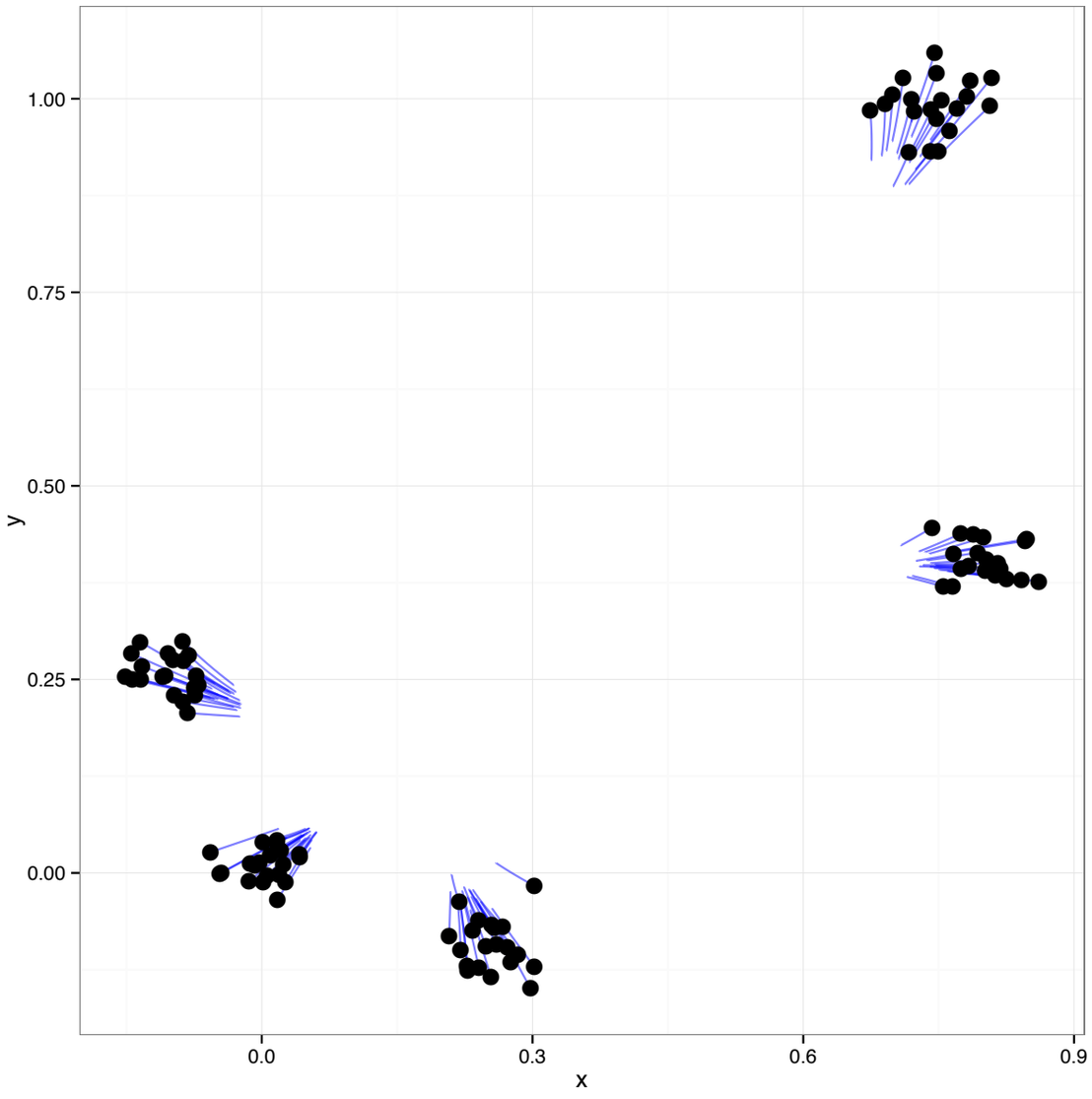
The Solution Path



γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma\sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

The Solution Path



γ

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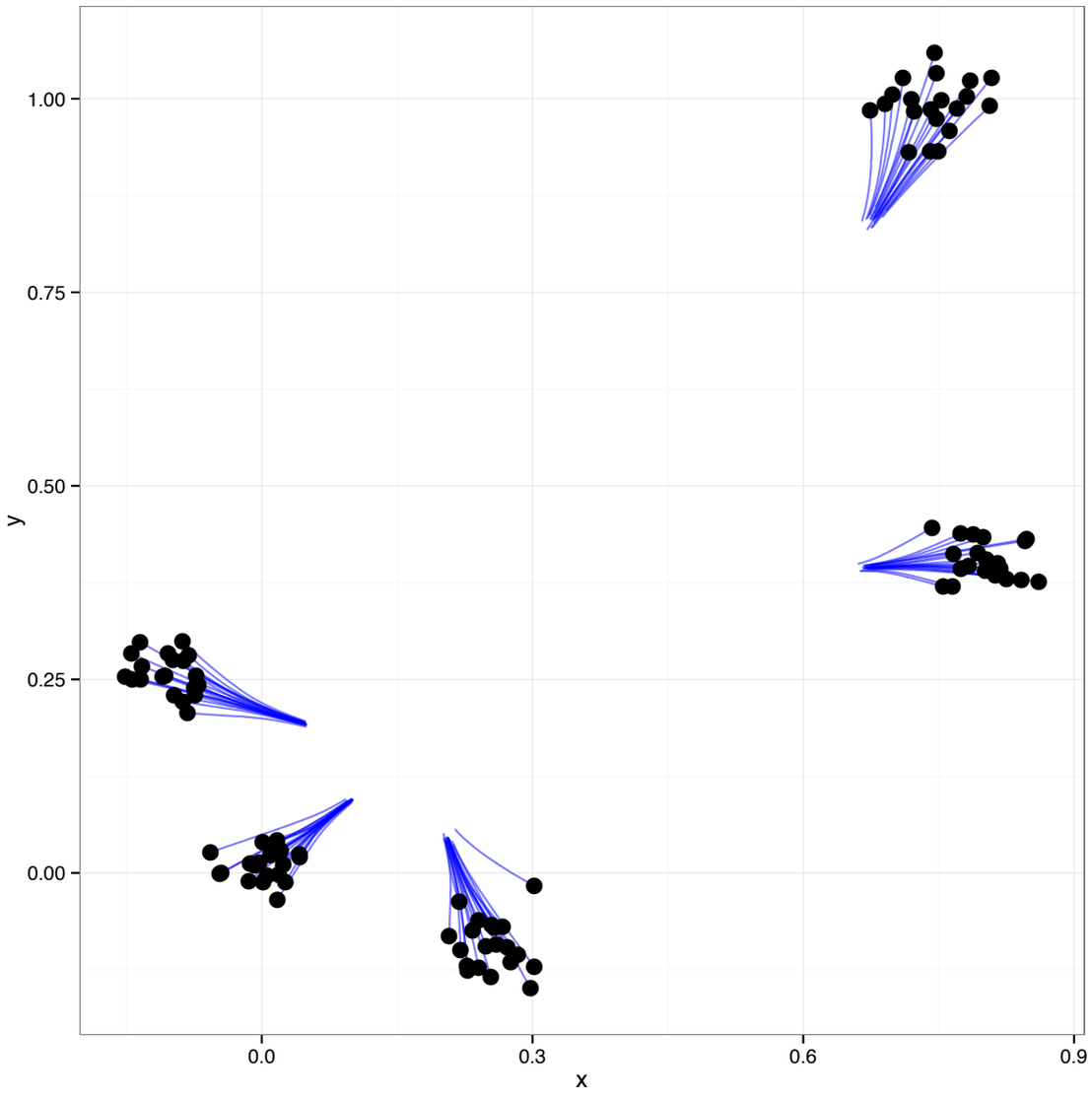
The Solution Path



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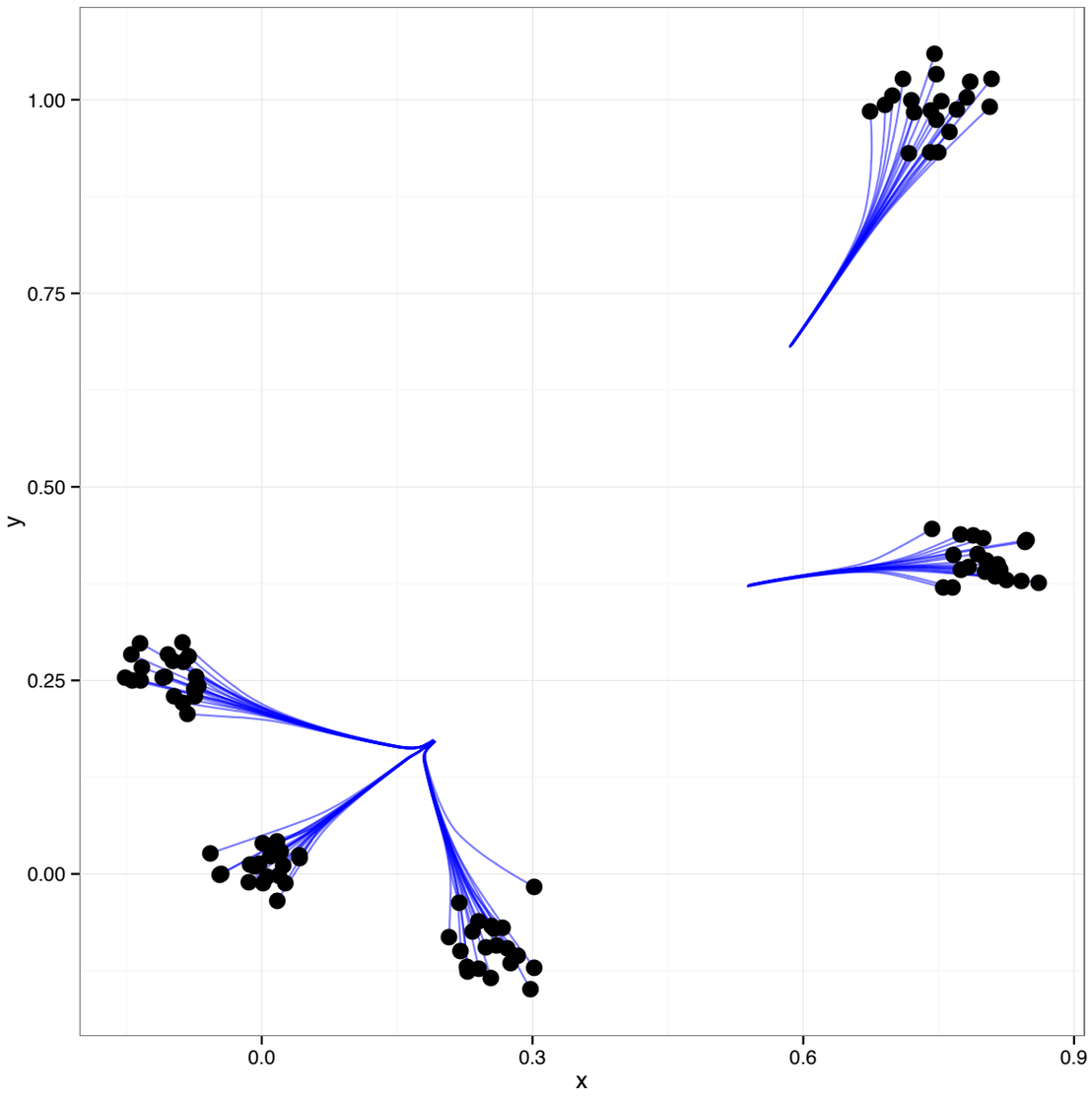
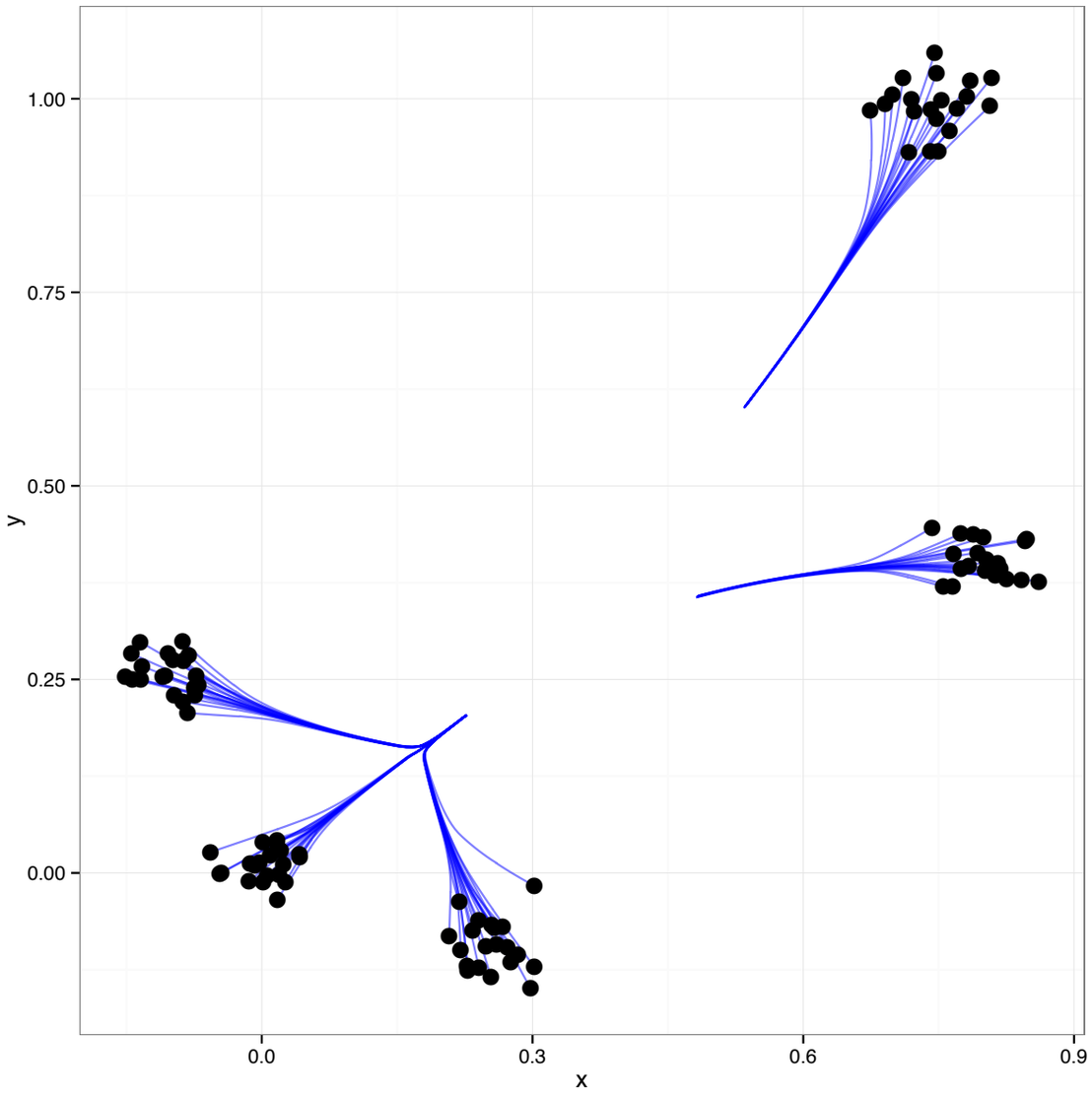
The Solution Path



γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

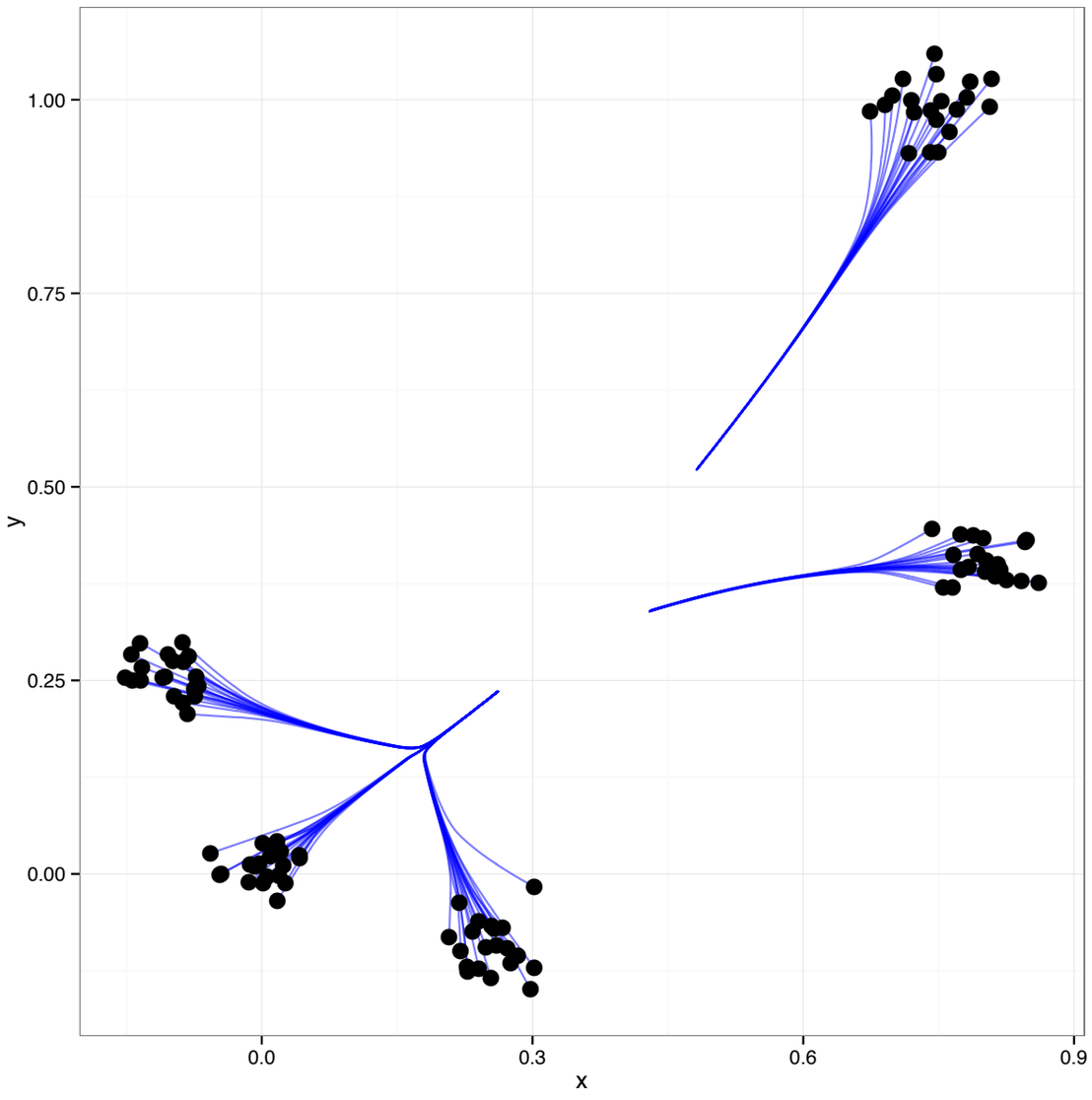
The Solution Path



γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

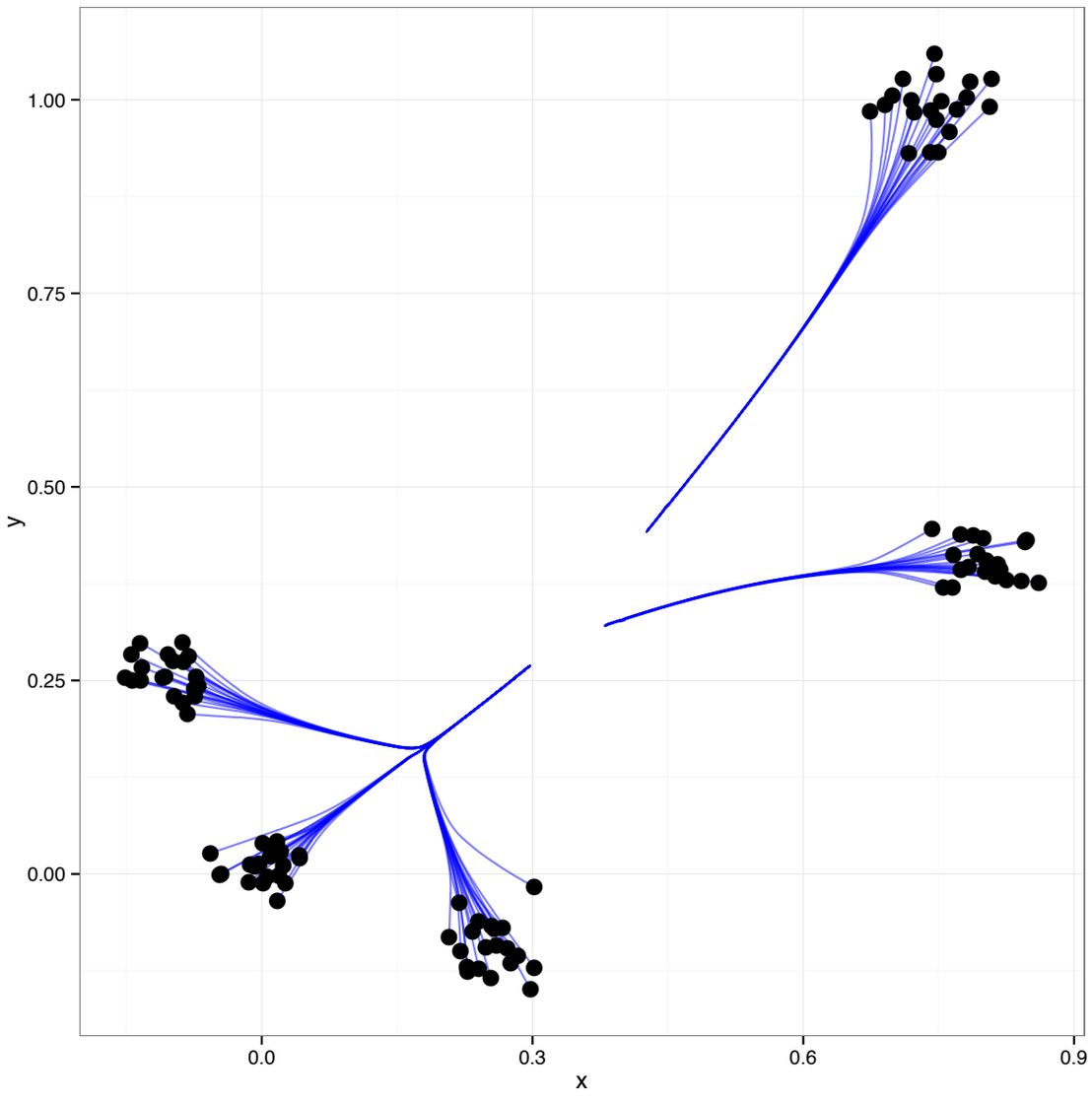
The Solution Path



γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

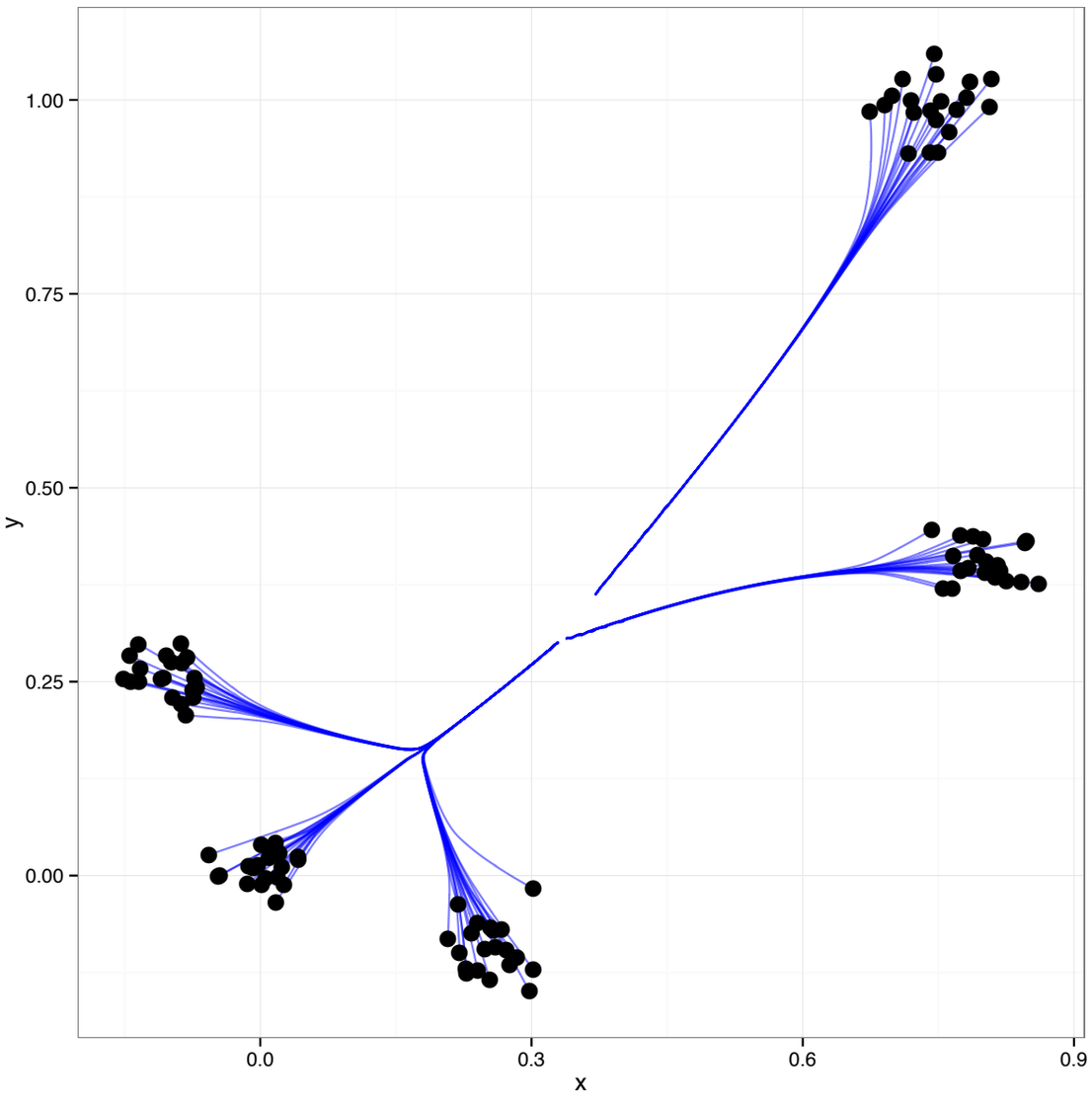
The Solution Path



γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

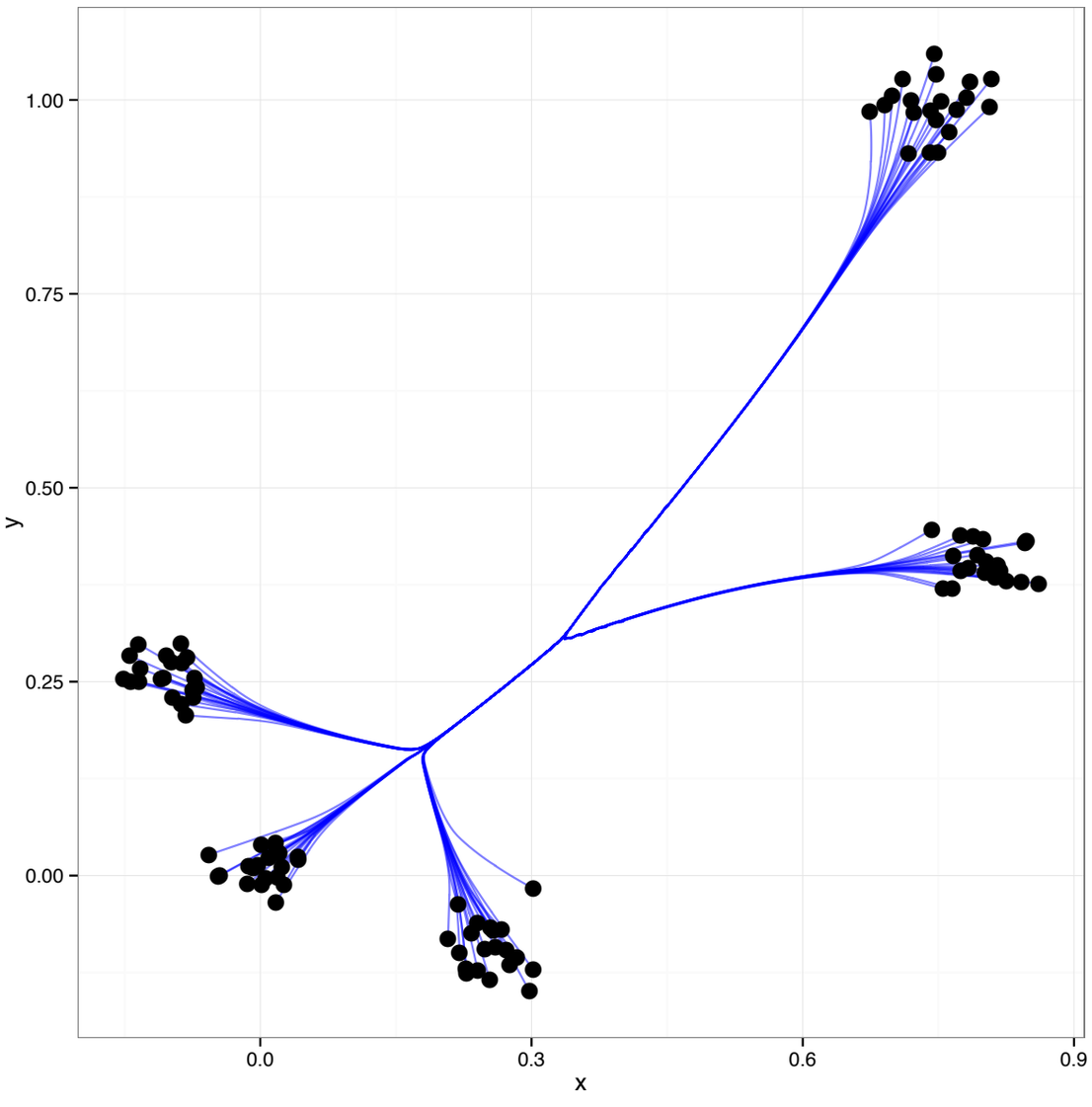
The Solution Path

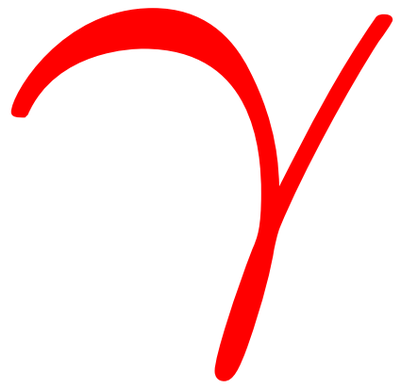


γ

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

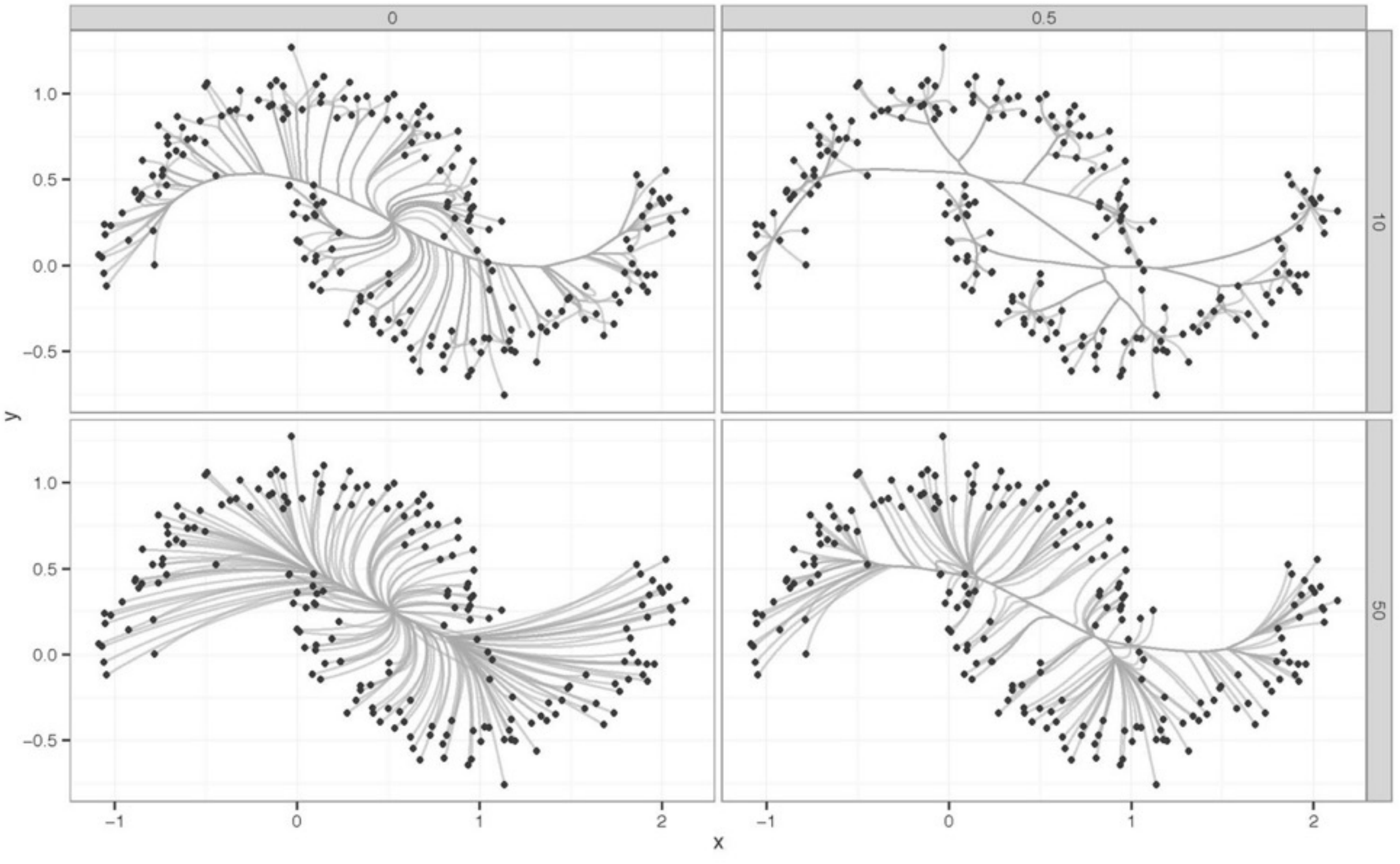
The Solution Path



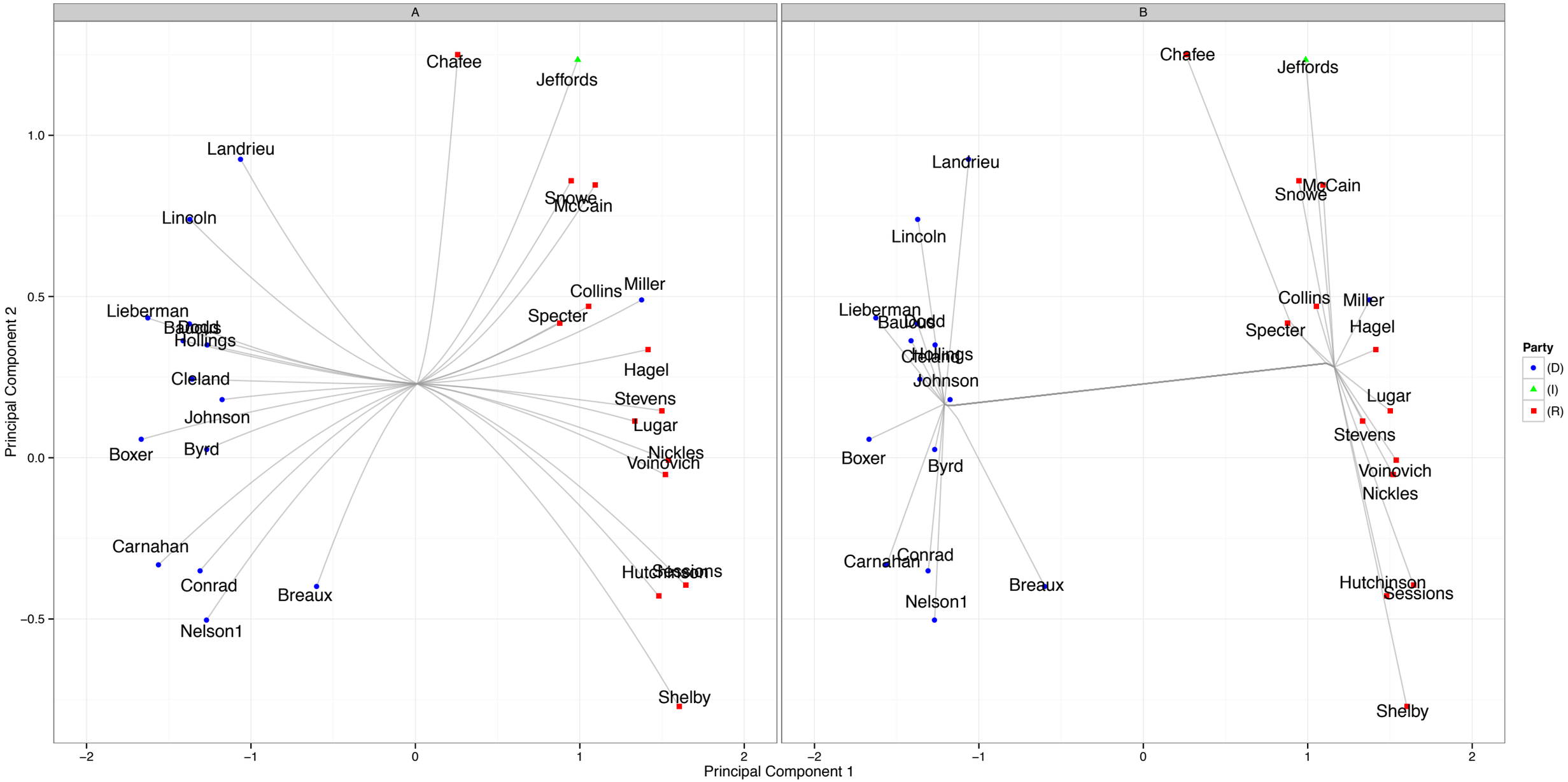


$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma\sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

Two Interlocking Half-Moons



Senate Voting



Apparently Non-Trivial Optimization Problem

Why is this hard to solve?

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

Apparently Non-Trivial Optimization Problem

Why is this hard to solve?

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

Nonsmooth? Not the issue

Apparently Non-Trivial Optimization Problem

Why is this hard to solve?

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

Affine transformation of u

Convex Clustering: Variable Split Version

$$\text{minimize } \frac{1}{2}\sum_{i=1}^{p}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \gamma\sum_{l} w_l\|\mathbf{v}_l\|$$

$$\text{subject to } \mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \mathbf{v}_l = \mathbf{0}$$

$$l = (l_1, l_2) \text{ with } l_1 < l_2.$$

ADMM Updates

$$
\begin{aligned}
\mathbf{u}_i &= \frac{1}{1+p\nu}\mathbf{y}_i + \frac{p\nu}{1+p\nu}\bar{\mathbf{x}} \\
\mathbf{y}_i &= \mathbf{x}_i + \sum_{l_1=i}[\boldsymbol{\lambda}_l + \nu\mathbf{v}_l] - \sum_{l_2=i}[\boldsymbol{\lambda}_l + \nu\mathbf{v}_l].
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{v}_l &= \arg\min_{\mathbf{v}} \frac{1}{2}\|\mathbf{v} - (\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l)\|_2^2 + \frac{\gamma w_l}{\nu}\|\mathbf{v}\| \\
&= \mathrm{prox}_{\sigma_l\|\cdot\|/\nu}(\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l),
\end{aligned}
$$

where $\sigma_l = \gamma w_l$.

$$
\boldsymbol{\lambda}_l = \boldsymbol{\lambda}_l + \nu(\mathbf{v}_l - \mathbf{u}_{l_1} + \mathbf{u}_{l_2}).
$$

AMA Updates

$$
\begin{aligned}
\mathbf{u}_i &= \frac{1}{1+p0}\mathbf{y}_i + \frac{p0}{1+p0}\bar{\mathbf{x}} \\
\mathbf{y}_i &= \mathbf{x}_i + \sum_{l_1=i}[\boldsymbol{\lambda}_l + 0\mathbf{v}_l] - \sum_{l_2=i}[\boldsymbol{\lambda}_l + 0\mathbf{v}_l].
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{v}_l &= \arg\min_{\mathbf{v}} \frac{1}{2}\|\mathbf{v} - (\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l)\|_2^2 + \frac{\gamma w_l}{\nu}\|\mathbf{v}\| \\
&= \mathrm{prox}_{\sigma_l\|\cdot\|/\nu}(\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l),
\end{aligned}
$$

where $\sigma_l = \gamma w_l$.

$$
\boldsymbol{\lambda}_l = \boldsymbol{\lambda}_l + \nu(\mathbf{v}_l - \mathbf{u}_{l_1} + \mathbf{u}_{l_2}).
$$

AMA Updates

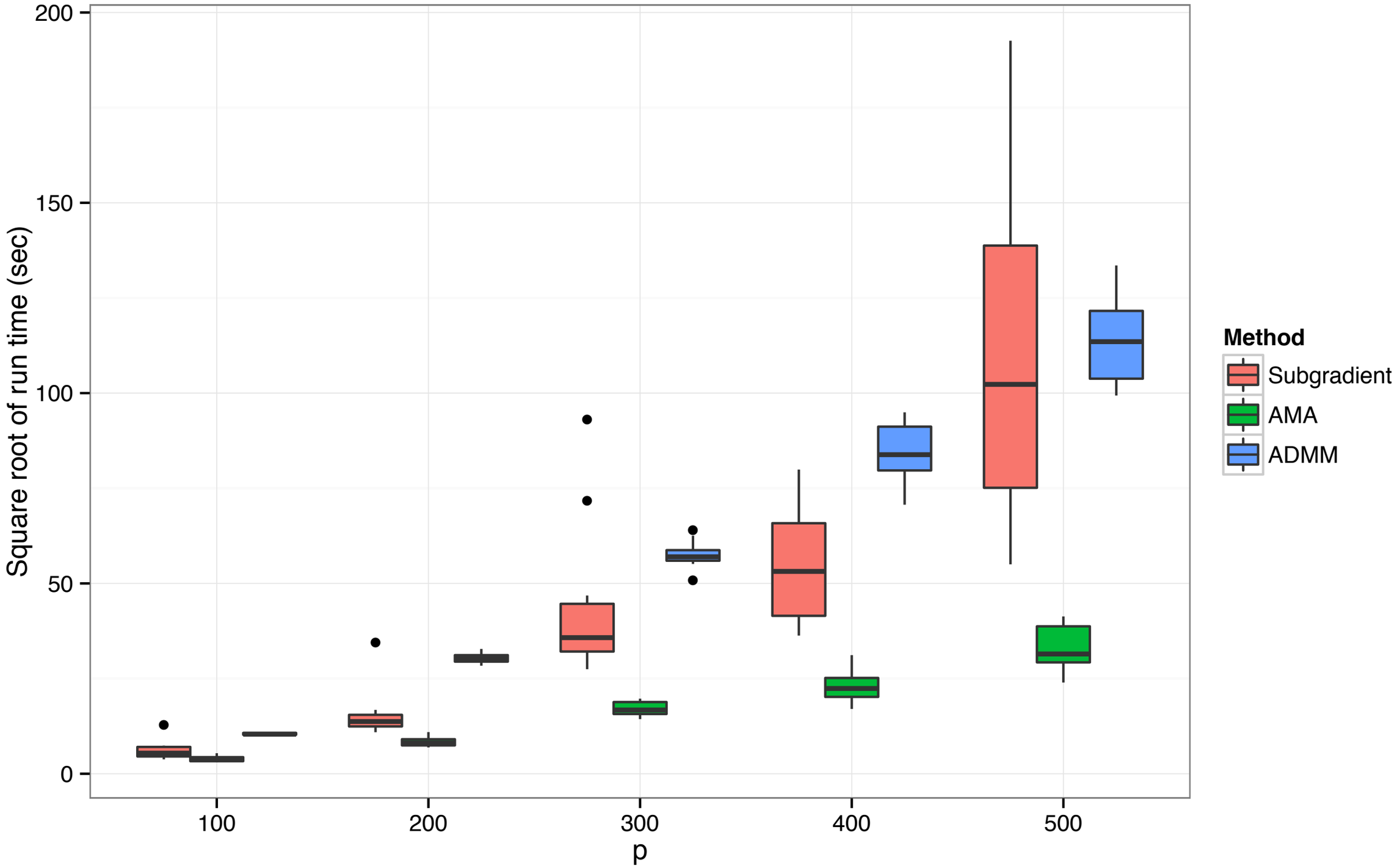
$$\mathbf{u}_i \quad = \quad \mathbf{x}_i + \sum_{l_1=i} \boldsymbol{\lambda}_l - \sum_{l_2=i} \boldsymbol{\lambda}_l$$

$$\begin{aligned}
\mathbf{v}_l &= \arg\min_{\mathbf{v}} \frac{1}{2}\|\mathbf{v} - (\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l)\|_2^2 + \frac{\gamma w_l}{\nu}\|\mathbf{v}\| \\
&= \mathrm{prox}_{\sigma_l\|\cdot\|/\nu}(\mathbf{u}_{l_1} - \mathbf{u}_{l_2} - \nu^{-1}\boldsymbol{\lambda}_l),
\end{aligned}$$

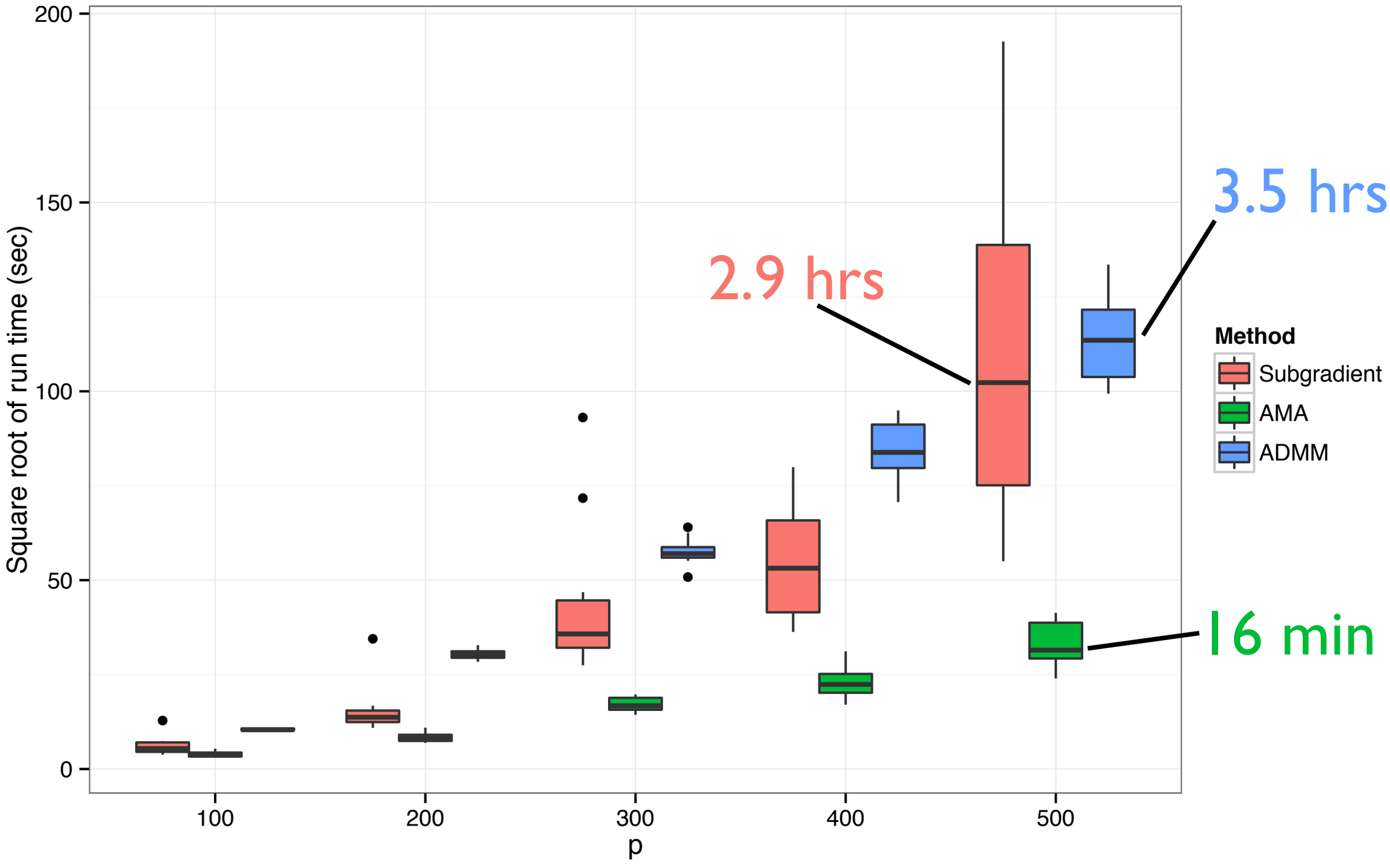
where $\sigma_l = \gamma w_l$.

$$\boldsymbol{\lambda}_l = \boldsymbol{\lambda}_l + \nu(\mathbf{v}_l - \mathbf{u}_{l_1} + \mathbf{u}_{l_2}).$$

What's the Difference?



What's the Difference?



ADMM versus AMA

$$\text{minimize } f(x) + g(y)$$
$$\text{subject to } Ax + By = c$$

ADMM:

- Pros: weaker conditions (f and g need to be closed and convex, problem needs to have a solution).
- Cons: will be slower (still scalable)

AMA:

- Pros: fast and scalable
- Cons: stronger conditions (f needs to be strongly convex)
- Tseng, P. (1991), "Applications of a Splitting Algorithm to Decomposition in Convex Programming and Variational Inequalities," SIAM Journal on Control and Optimization, 29, 119-138.

Summary

Duality is useful for

1. Checking correctness of a solution & debugging your code
2. Designing an alternative algorithm for solving an equivalent dual problem.