Lecture 14: Stochastic Gradient Descent

-What do we use in practice?



Machine Learning Problems

- Given data: $\{(x_i, y_i)\}_{i=1}^n$ $x_i \in \mathbb{R}^d$ $y_i \in \mathbb{R}$
- Learning a model's parameters: $\frac{1}{n} \sum_{i=1}^{n} \ell_i(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_w(x_i), y_i)$
- Gradient Descent (GD): one update takes cdn operations/time for some constant c>0 $w_{t+1} \leftarrow w_t - \eta \frac{1}{n} \sum_{i=1}^n \nabla \mathcal{E}_i(w_t)$

• Stochastic Gradient Descent (SGD): one update takes
$$cd$$
 operations/time

$$w_{t+1} \leftarrow w_t - \eta \nabla \mathcal{C}_{I_t}(w_t)$$
 $I_t \text{ drawn uniform at random from } \{1, \dots, n\}$

SGD is an unbiased estimate of the GD

$$\mathbb{E}[\nabla \ell_{I_t}(w)] = \sum_{i=1}^n \mathbb{P}(I_t = i) \nabla \ell_i(w) = \frac{1}{n} \sum_{i=1}^n \nabla \ell_i(w)$$

Stochastic Gradient Descent

Theorem Let $w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w) \Big|_{w=w_t}$ I_t drawn uniform at random from $\{1, \dots, n\}$ If $||w_0 - w_*||_2^2 \le R$ and $\sup_i \max_i ||\nabla \ell_i(w)||_2^2 \le G$ after T steps of SGD with stepsize η , we achieve $\mathbb{E}[\ell(\overline{w}) - \ell(w_*)] \leq \frac{R}{2T\eta} + \frac{\eta G}{2} \qquad \text{Voriance} \qquad \frac{0.2}{0.3}$ $\text{The optimal stepsize,} \qquad \min_{\eta>0} \frac{R}{2T\eta} + \frac{\eta G}{2} = \sqrt{\frac{RG}{T}} \qquad \text{for} \qquad \eta = \sqrt{\frac{R}{GT}}$ Selecting the optimal stepsize,

$$\overline{w} = \frac{1}{T} \sum_{t=1}^{T} w_t$$

Convergence rate: $O\left(\frac{1}{\sqrt{T}}\right)$

(Fixed optimal step size)

$$-\frac{R}{2T\eta^2} + \frac{G}{2} = 0$$

(In practice use last iterate)

Taking the derivative of RHS to zero

We want to show that

Proof

$$\mathcal{E}(w_*)$$

 $\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=0}^{T}w_{t}\right)-\ell(w_{*})\right] \leq \mathbb{E}\left[\frac{1}{T}\sum_{t=0}^{T}\ell(w_{t})-\ell(w_{*})\right]$ and Jensen's inequality (3 slides later) $\leq \frac{1}{T} \sum_{t=0}^{T} \mathbb{E} \left[\ell(w_t) - \ell(w_*) \right]$ Follows from linearity of expectation

$$\leq \frac{R}{2T\eta} + \frac{\eta G}{2}$$

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

$$= \mathbb{E}[||w_{t+1} - w_*||_2^2] + \mathcal{N}^2 \mathbb{E}[|\nabla_{I_t}(w_t)|^2]$$

Dust (terate VR(We) (We-Wa) > R(Ve)-R(Wa)

R(We)= 1 7 li(We)

Noise Grad.
$$=0(\eta^2)$$

$$\leq \eta^2 G$$

Follows from convexity of $\mathcal{E}(\cdot)$

We are left to show this

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

$$\leq \mathbb{E}[||w_t - w_*||_2^2] + \eta^2 G - 2\eta(\ell(w_t))$$

$$\leq \mathbb{E}[\|w_t - w_*\|_2^2] + \eta^2 G - 2\eta(\ell(w_t) - \ell(w_*))$$

$$|\mathcal{L}(w_e) - \mathcal{L}(w_*)| \leq \frac{1}{29} \left(\mathbb{E}[|w_e - w_*|]_2^2 \right] - \mathbb{E}[|w_{e_{11}} - w_*|]_2^2 + 9^2 G$$

$$= \frac{1}{29} \left(\mathbb{E}[|w_e - w_*|]_2^2 \right) - \mathbb{E}[|w_{e_{11}} - w_*|]_2^2 + \mathbb{E}[|w_$$

$$\sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \le \frac{R}{2\eta} + \frac{T\eta G}{2}$$

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

$$= \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] + \eta^2 \mathbb{E}[||\nabla \ell_{I_t}(w_t)||_2^2]$$

$$\leq \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\ell(w_t) - \ell(w_*)] + \eta^2 G$$

$$\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] = \mathbb{E}[\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*) | I_1, w_1, \dots, I_{t-1}, w_{t-1}]]$$

$$= \mathbb{E}[\nabla \ell(w_t)^T (w_t - w_*)]$$

$$\geq \mathbb{E}[\ell(w_t) - \ell(w_*)]$$

$$\sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \le \frac{1}{2\eta} \left(\mathbb{E}[||w_1 - w_*||_2^2] - \mathbb{E}[||w_{T+1} - w_*||_2^2] + T\eta^2 G \right)$$

$$\le \frac{R}{2\eta} + \frac{T\eta G}{2}$$

Jensen's inequality:

We have shown:
$$\sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \le \frac{R}{2\eta} + \frac{T\eta G}{2}$$
Jensen's inequality











- - Jensen's inequality

- $\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T}w_{t}\right)-\ell(w_{*})\right] \leq \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[\ell(w_{t})-\ell(w_{*})]$

 $\leq \frac{R}{2nT} + \frac{\eta G}{2}$

 $\mathscr{E}(w)$

For any $\{w_1, ..., w_T\}$ and a convex function $\mathcal{C}(\cdot)$, we have

 $\mathscr{E}\left(\frac{1}{T}\sum_{t=1}^{T}w_{t}\right)\leq\frac{1}{T}\sum_{t=1}^{T}\mathscr{E}(w_{t})$

Mini-batch SGD

- Instead of one iterate, average B stochastic gradient together
- Advantages:
 - Smaller variance: the variance of the stochastic gradient is smaller by a factor of $1/\sqrt{B}$
 - Parallelization: each gradient in the mini-batch can be computed in parallel
 - If you have regularizer, $\frac{1}{n}\sum_{i=1}^n \mathscr{C}_i(w) + r(w)$, then update with the stochastic gradient of the loss and gradient of the regularizer

Questions?

Lecture 14: Coordinate Descent

- How to solve non-smooth optimization like Lasso?

$$\hat{w}_{\text{Lasso}} = \arg\min_{w \in \mathbb{R}^d} \ ||\mathbf{y} - \mathbf{X}w||_2^2 + \lambda ||w||_1$$

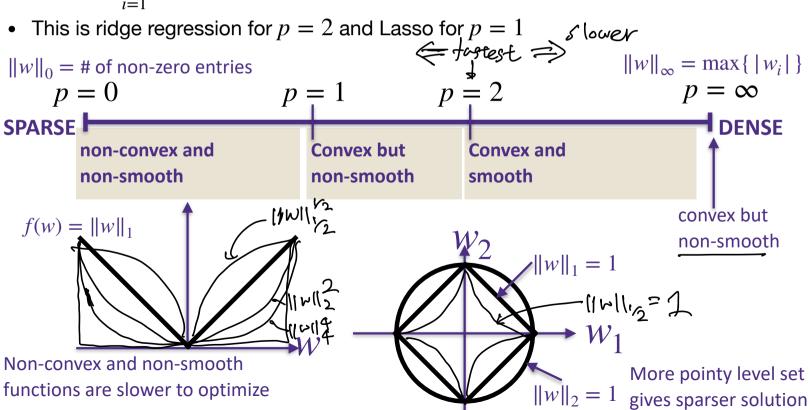


Sparsity/Complexity tradeoff

- \mathscr{C}_p -norm of a vector is defined as $\|w\|_p \triangleq \left(|w_1|^p + |w_2|^p + \dots + |w_d|^p \right)^{1/p}$
- Consider regularized least squares problem of minimizing

$$\mathcal{L}(w) = \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \lambda \|w\|_p^p$$

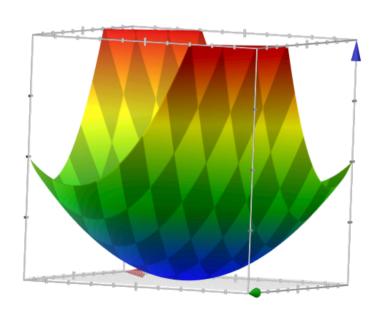
- This is ridge regression for p=2 and Lasso for p=1

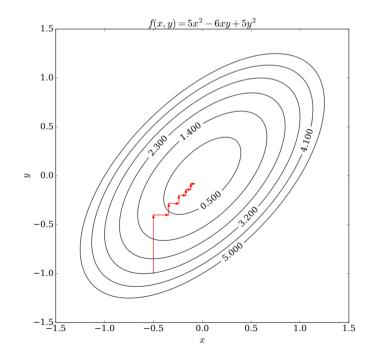


Optimization: how do we solve Lasso?

- among many methods to find the solution, we will learn coordinate descent method
- as an illustrating example, we show coordinate descent updates on finding the minimum of a very simple function:

$$f(x,y) = 5x^2 - 6xy + 5y^2$$

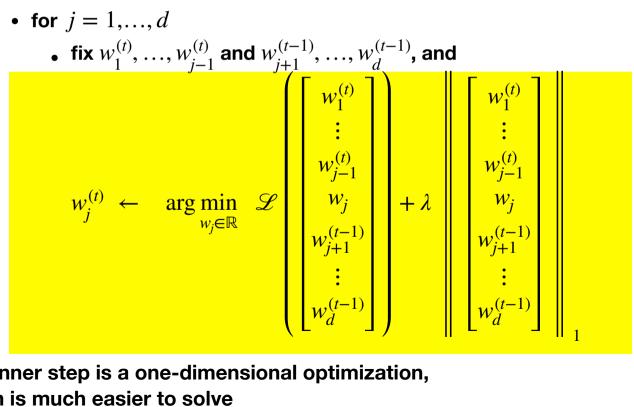




How do we solve Lasso: min $\mathcal{L}(w) + \lambda ||w||_1$?

W

- Coordinate descent
 - input: training data $S_{
 m train}$, max # of iterations T
 - initialize: $w^{(0)} = \mathbf{0} \in \mathbb{R}^d$
 - for t = 1, ..., T
 - for j = 1,...,d
 - fix $w_1^{(t)}, ..., w_{j-1}^{(t)}$ and $w_{j+1}^{(t-1)}, ..., w_d^{(t-1)}$, and



 This inner step is a one-dimensional optimization, which is much easier to solve

Coordinate descent for (un-regularized) linear regression

• let us understand what coordinate descent does on a simpler problem of linear least squares, which minimizes

$$\operatorname{minimize}_{w} \mathcal{L}(w) = \|\mathbf{X}w - \mathbf{y}\|_{2}^{2}$$

- note that we know that the optimal solution is $\hat{w}_{LS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ so we do not need to run any optimization algorithm
- we are solving this problem with **coordinate descent** as a starting example to learn how coordinate descent works
- the main challenge we address is, how do we update $w_i^{(t)} \in \mathbb{R}$?
- let us derive an **analytical rule** (i.e., closed form solution) for updating $w_j^{(t)}$, which generalizes to the case when we have Lasso regularizer.

Coordinate descent for (un-regularized) linear regression

We consider the case when updating coordinate j = 1

$$\min_{w_{1} \in \mathbb{R}} \|\mathbf{X}w - \mathbf{y}\|_{2}^{2} = \min_{w_{1} \in \mathbb{R}} (aw_{1} - b)^{2} + \text{constant}$$

$$\|\mathbf{X}w - \mathbf{y}\|_{2}^{2} = \|\mathbf{x}_{1} \cdot \mathbf{w}_{1} - (\mathbf{y} - \mathbf{x}_{1} \cdot \mathbf{w}_{1})\|_{2}^{2}$$

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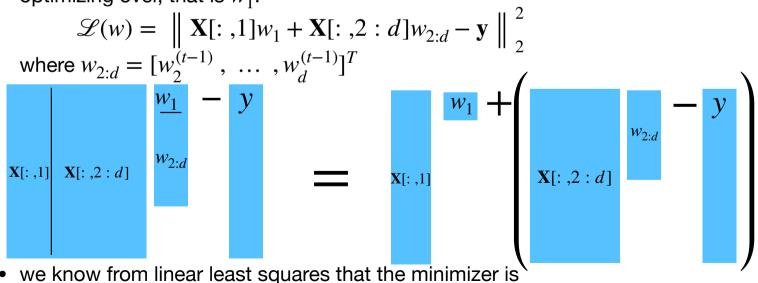
$$= \|\mathbf{x}_{1} \cdot \mathbf{w}_{1} - (\mathbf{y} - \mathbf{x}_{1} \cdot \mathbf{w}_{1})\|_{2}$$

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$$= \|\mathbf{x}_{1}$$

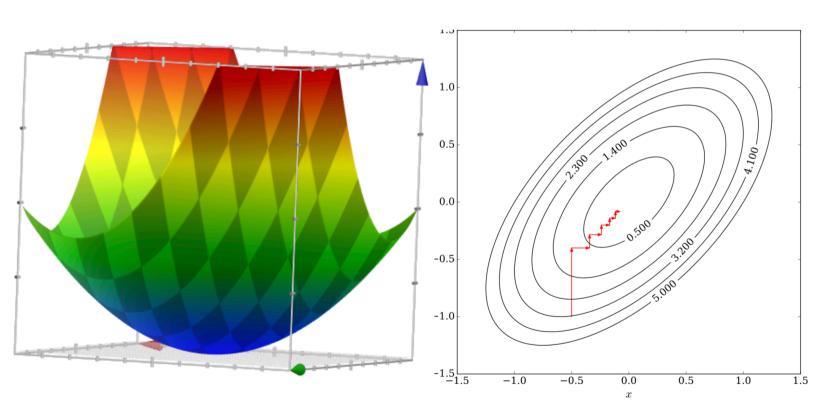
Coordinate descent for (un-regularized) linear regression

- we will study the case j = 1, for now (other cases are almost identical)
- when updating $w_1^{(t)}$, recall that $w_1^{(t)} \leftarrow \arg\min_{w_1} \|\mathbf{X}w \mathbf{y}\|_2^2$ where $w = [w_1, \ w_2^{(t-1)}, \ \dots, w_d^{(t-1)}]^T$
- first step is to write the objective function in terms of the variable we are optimizing over, that is w_1 :



 $w_1^{(t)} \leftarrow (\mathbf{X}[:,1]^T \mathbf{X}[:,1])^{-1} \mathbf{X}[:,1]^T (\mathbf{y} - \mathbf{X}[:,2:d] w_{2:d})$

Coordinate descent applied to a quadratic loss



Coordinate descent for Lasso

- let us apply coordinate descent on Lasso, which minimizes $\min_{w} \mathcal{L}(w) + \lambda ||w||_1 = ||\mathbf{X}w \mathbf{y}||_2^2 + \lambda ||w||_1$
- the goal is to derive an **analytical rule** for updating $w_j^{(t)}$'s
- let us first write the update rule explicitly for $W_1^{(t)}$
 - first step is to write the loss in terms of w_1

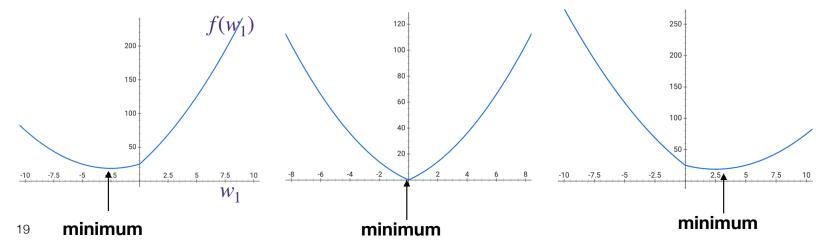
$$\|\mathbf{X}[:,1]w_1 - (\mathbf{y} - \mathbf{X}[:,2:d]w_{2:d})\|_2^2 + \lambda((w_1) + (w_2:d))\|_2^2 + \lambda((w_1) + (w_2:d))\|_2^2$$

• hence, the coordinate descent update boils down to $(\omega W, -6)^2$

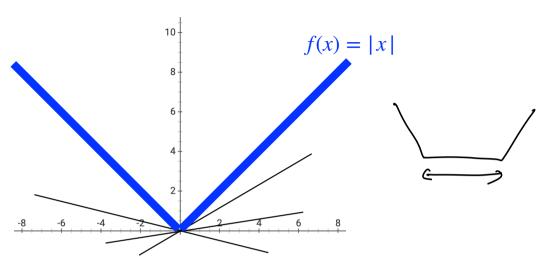
$$w_1^{(t)} \leftarrow \arg\min_{w_1} \left\| \mathbf{X}[:,1]w_1 - \left(\mathbf{y} - \mathbf{X}[:,2:d] w_{2:d}^{(t-1)} \right) \right\|_2^2 + \lambda |w_1|$$

Convexity

- to find the minimizer of $f(w_1)$, let's study some properties
- for simplicity, we represent the objective function as $f(w_1) = (aw_1 b)^2 + \lambda |w_1|$
- this function is
 - convex, and
 - non-differentiable
- depending on the values of a, b, and λ , the function looks like one of the three below



Convexity



- for a **non-differentiable** function, gradient is not defined at some points, for example at x = 0 for f(x) = |x|
- at such points, sub-gradient plays the role of gradient
 - sub-gradient at a differentiable point is the same as the gradient
 - sub-gradient at a non-differentiable point is a set of vector satisfying

$$\partial f(x) = \left\{ g \in \mathbb{R}^d \mid f(y) \ge f(x) + g^T(y - x), \text{ for all } y \in \mathbb{R}^d \right\}$$

• for example, sub-gradient of $|\cdot|$ is $\partial |x| = \begin{cases} +1 & \text{for } x > 0 \\ [-1,1] & \text{for } x = 0 \\ -1 & \text{for } x < 0 \end{cases}$

Computing the sub-gradient

$$w_{1}^{(t)} = \arg\min_{w_{1} \in \mathbb{R}} \left\| \mathbf{X}[:,1]w_{1} - \left(\mathbf{y} - \mathbf{X}[:,2:d]w_{2:d}^{(t-1)}\right) \right\|_{2}^{2} + \lambda |w_{1}|$$

$$f(w_{1}) = (aw_{1} - b)^{2} + \lambda |w_{1}| + \text{constant} \qquad \text{Where } a = \sqrt{\mathbf{X}[:,1]^{T}\mathbf{X}[:,1]}, \text{ and}$$

$$b = \frac{\mathbf{X}[:,1]^{T}(\mathbf{y} - \mathbf{X}[:,2:d]w_{2:d}^{(t-1)})}{\sqrt{\mathbf{X}[:,1]^{T}\mathbf{X}[:,1]}}$$

$$\frac{\partial f(w_i)}{\partial f(w_i)} = 2\alpha(\alpha w_i - b) + \lambda \cdot \frac{\partial f(w_i)}{\partial f(w_i)} \\
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Computing the sub-gradient

$$w_1^{(t)} = \arg\min_{w_1 \in \mathbb{R}} \left\| \mathbf{X}[:,1] w_1 - \left(\mathbf{y} - \mathbf{X}[:,2:d] w_{2:d}^{(t-1)} \right) \right\|_2^2 + \lambda |w_1|$$

• We have $f(w_1) = (aw_1 - b)^2 + \lambda |w_1| + \text{constants}$, with

•
$$a = \sqrt{\mathbf{X}[:,1]^T \mathbf{X}[:,1]}$$
, and
$$b = \frac{\mathbf{X}[:,1]^T (\mathbf{y} - \mathbf{X}[:,2:d] w_{2:d}^{(t-1)})}{\sqrt{\mathbf{X}[:,1]^T \mathbf{X}[:,1]}}$$

$$\sqrt{\mathbf{X}}[:,1]^T\mathbf{X}[:,1]$$

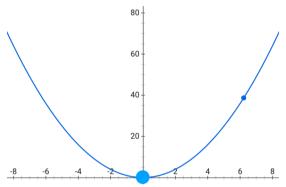
• $f(w_1)$ is non-differentiable, and its sub-gradient is

$$\partial f(w_1) = (2a(aw_1 - b) + \lambda \partial |w_1|)$$

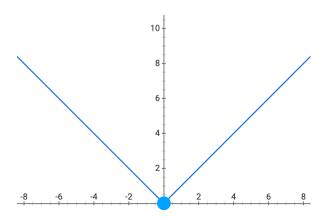
$$= \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0\\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0\\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

How do we find the minima?

 for convex differentiable functions, the minimum is achieved at points where gradient is zero



 for convex non-differentiable functions, the minimum is achieved at points where sub-gradient includes zero



• the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

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 considering all three cases, we get the following update rule by setting the sub-gradient to zero

$$w_1^{(t)} \leftarrow \begin{cases} \frac{b}{a} - \frac{\lambda}{2a^2} & \text{for } 2ab > \lambda \\ 0 & \text{for } -\lambda \le 2ab \le \lambda \iff \frac{-\lambda}{2a^2} \le \frac{b}{a} \le \frac{\lambda}{2a^2} \\ \frac{b}{a} + \frac{\lambda}{2a^2} & \text{for } \lambda < -2ab \end{cases}$$

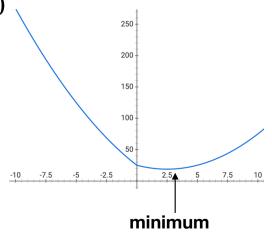
How do we find the minimizer?

 $\bullet \;$ the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

- case 1:
 - $2a(aw_1 b) + \lambda = 0$ for some $w_1 > 0$
 - this happens when $w_1 = \frac{-\lambda + 2ab}{2a^2} > 0$ box
 - hence, $w_1^{(t)} \leftarrow \frac{b}{a} \frac{\lambda}{2a^2},$



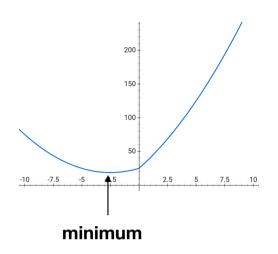


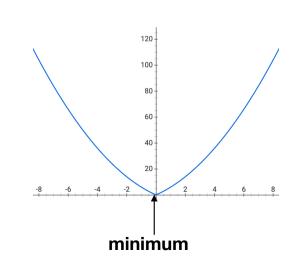
- case 2:
 - $2a(aw_1 b) \lambda = 0$ for some $w_1 < 0$
 - this happens when $w_1 = \frac{\lambda + 2ab}{2a^2} < 0$
 - hence, $w_1^{(t)} \leftarrow \frac{b}{a} + \frac{\lambda}{2a^2},$

if
$$\lambda < -2ab$$

- case 3:
 - $0 \in [-2ab \lambda, -2ab + \lambda]$
 - and $w_1 = 0$
 - hence, $w_1^{(t)} \leftarrow 0$,

if
$$-\lambda \le 2ab \le \lambda$$





Coordinate descent on Lasso

30

considering all three cases, we get the following update rule by setting the sub-gradient to zero

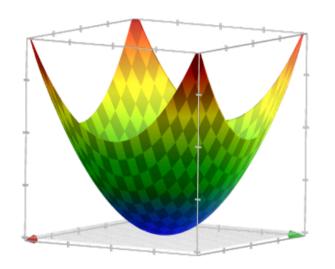
$$w_1^{(t)} \leftarrow \begin{cases} \frac{b}{a} - \frac{\lambda}{2a^2} & \text{for } 2ab > \lambda \\ 0 & \text{for } -\lambda \le 2ab \le \lambda \\ \frac{b}{a} + \frac{\lambda}{2a^2} & \text{for } \lambda < -2ab \end{cases}$$

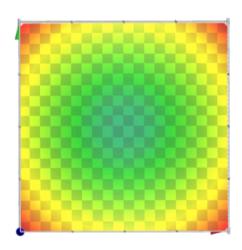
where
$$a = \sqrt{\mathbf{X}[:,1]^T \mathbf{X}[:,1]}$$
, and $b = \frac{\mathbf{X}[:,1]^T (\mathbf{y} - \mathbf{X}[:,2:d] w_{-1})}{\sqrt{\mathbf{X}[:,1]^T \mathbf{X}[:,1]}}$

minimum

When does coordinate descent work?

• Consider minimizing a **differentiable convex** function f(x), then coordinate descent converges to the global minima

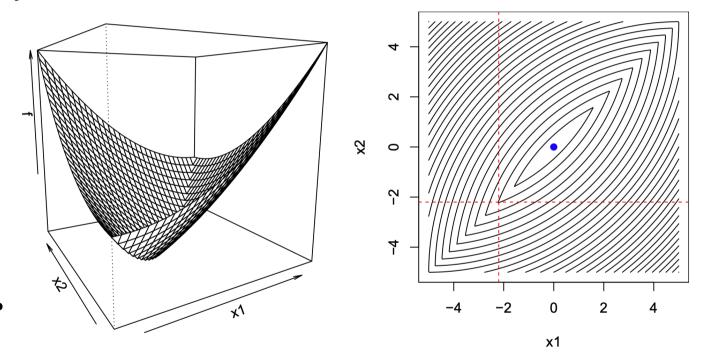




- when coordinate descent has stopped, that means $\frac{\partial f(x)}{\partial x_i} = 0 \text{ for all } j \in \{1, ..., d\}$
- this implies that the gradient $\nabla_x f(x) = 0$, which happens only at minimum

When does coordinate descent work?

• Consider minimizing a **non-differentiable convex** function f(x), then coordinate descent can get stuck

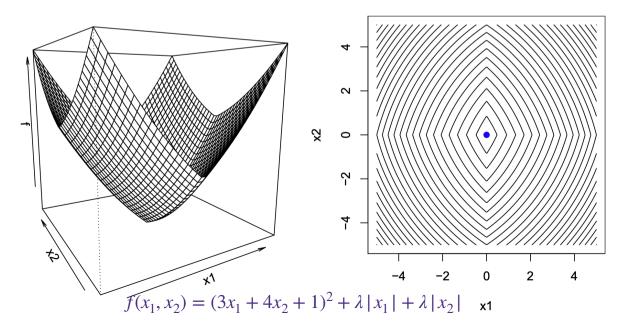


$$f(x_1, x_2) = (3x_1 + 4x_2 + 1)^2 + \lambda |x_1 - x_2|$$

When does coordinate descent work?

- then how can coordinate descent find optimal solution for Lasso?
- consider minimizing a **non-differentiable convex** function but has a structure of $f(x) = g(x) + \sum_{j=1}^d h_j(x_j)$, with differentiable convex

function g(x) and coordinate-wise non-differentiable convex functions $h_j(x_i)$'s, then coordinate descent converges to the global minima



Questions?