

Gradient Descent

Minimizing loss functions

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Minimizing the loss: How we train (many) models

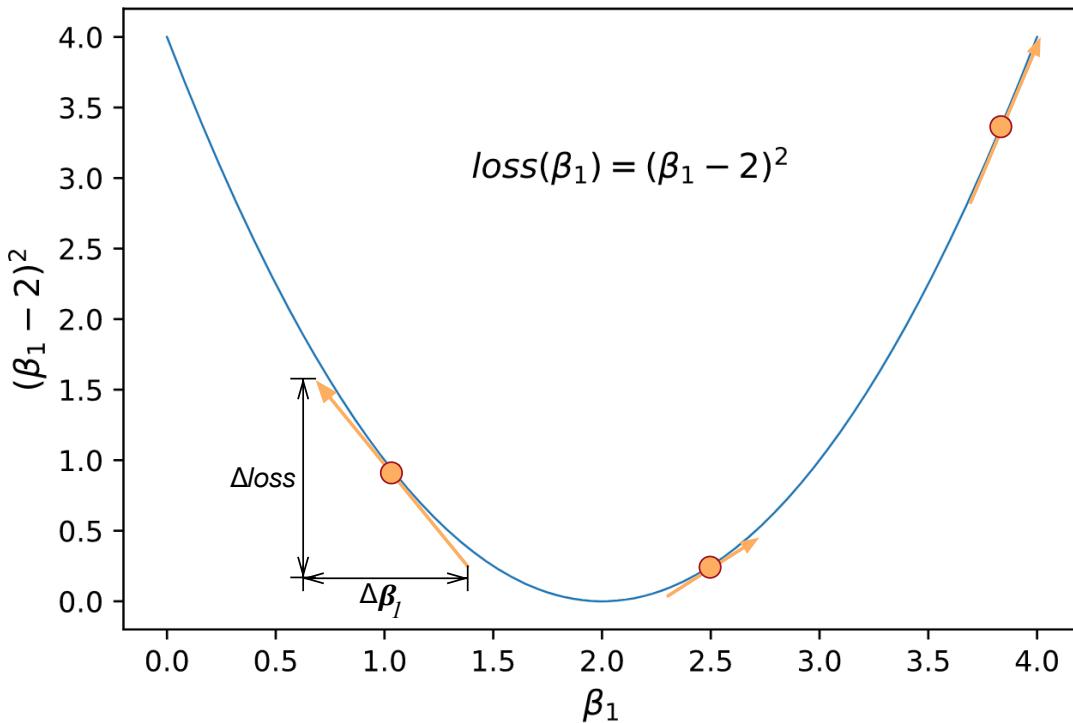
- We need a way to find β such that: $\arg \min_{\beta} \mathcal{L}(\beta)$
- Could try random β vectors and choose the β with lowest loss
- Or, better yet, choose a random β and then tweak with some $\Delta\beta$ in the downhill loss direction until any tweak would increase loss

$$\beta^{(t+1)} = \beta^{(t)} + \Delta\beta^{(t)}$$

- We use information about the loss function in the neighborhood of current β to decide which direction shifts towards smaller loss
- When loss goes up or doesn't change, we're done

How do we pick a direction to move?

- Use information (*gradient*) from loss function in vicinity of current β_1



- Derivative/slope of loss(β_1) is $2(\beta_1 - 2)$, which points in direction of increased loss (up)
- What is derivative of loss at $\beta_1=2$?
- Direction of min loss is opposite/negative of derivative
- Derivative also has magnitude, which is bigger when slope is steeper
- **How to move:** $\beta_1 = \beta_1 - \text{slope}$

Taking steps in right direction

- Direction of min loss is opposite of derivative so let's step in negative of derivative and scale it with a learning rate η :

$$\beta^{(t+1)} = \beta^{(t)} - \eta \frac{d}{d\beta} \mathcal{L}(\beta^{(t)})$$

```
while not_converged:  
    b = b - rate * gradient(b)
```

- We will always converge if learning rate is small enough

Python gradient descent implementation

- First define a simple loss function and its gradient:

```
def f(b) : return (b-2)**2  
def gradient(b): return 2*(b-2)
```

- Then, pick a random starting point and pick a learning rate

```
b = np.random.uniform(0,4)  
rate = .2
```

- Loop until we've made some progress or until $\text{gradient}(b) == 0$

```
for t in range(10): # for awhile  
    b = b - rate * gradient(b)
```

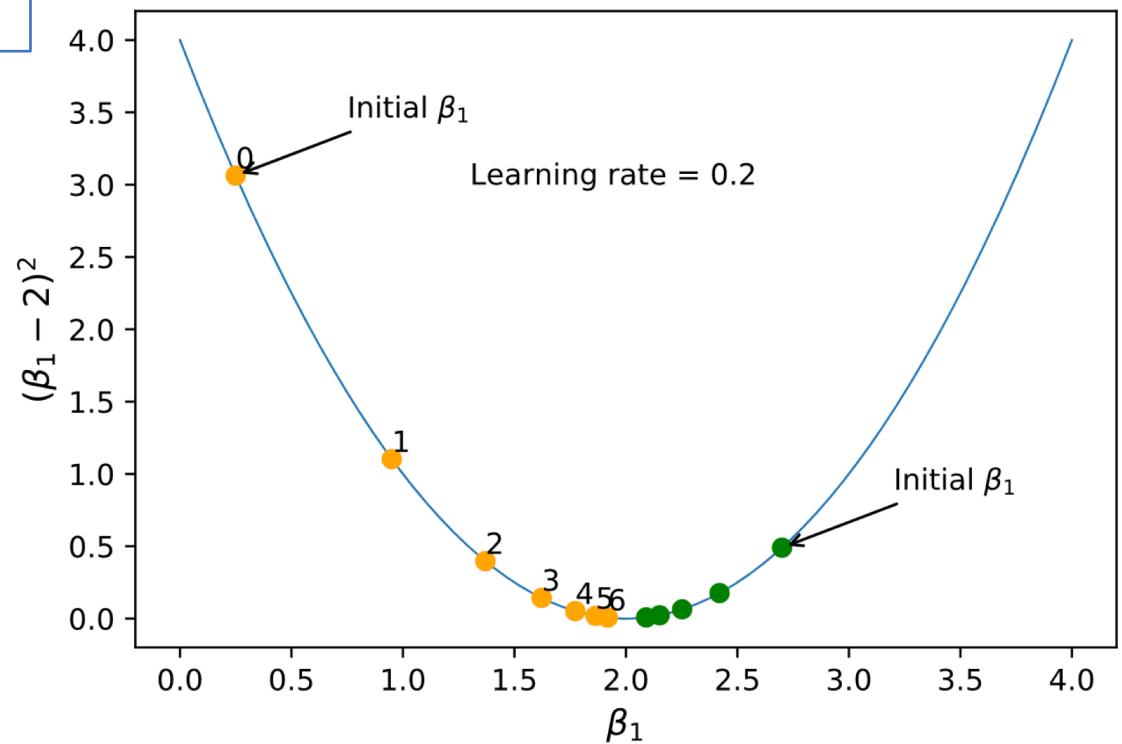
See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-gradient-descent.ipynb>

Sample 1D gradient descent run

```
for t in range(7):  
    b = b - 0.2 * gradient(b)
```

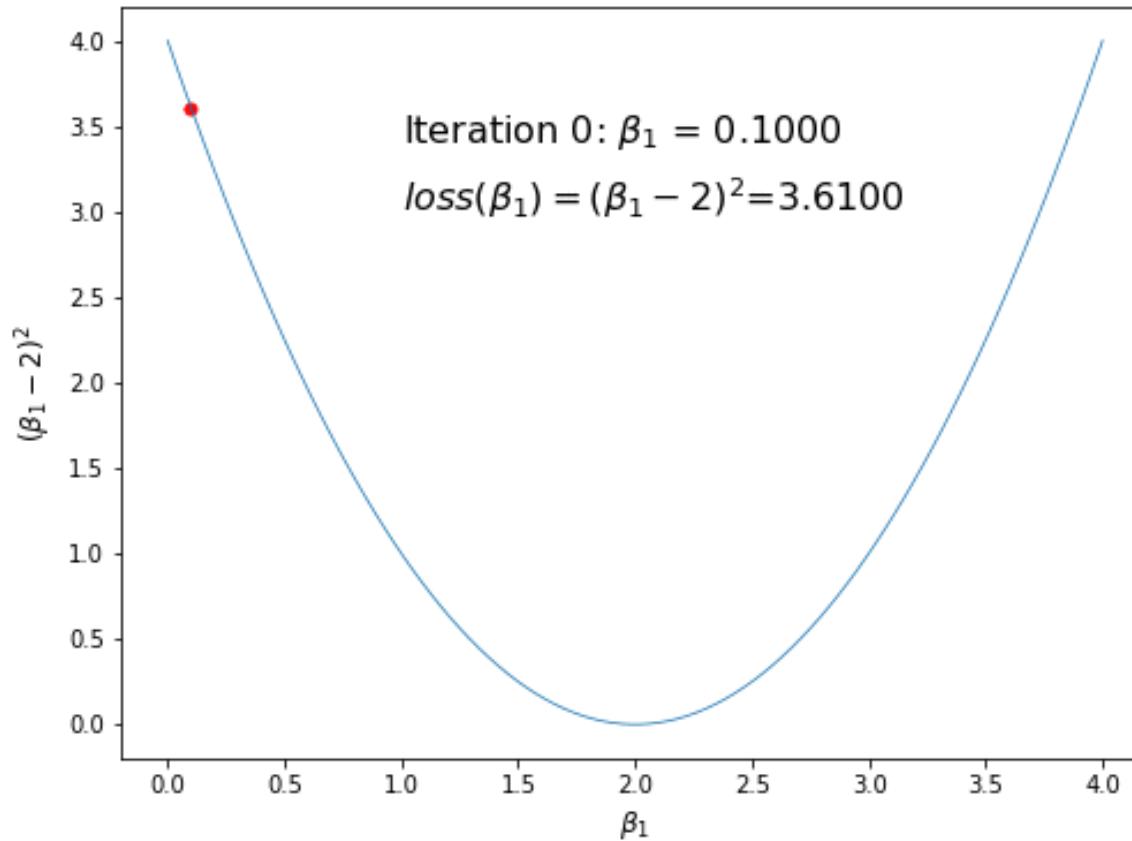
	beta_1	loss
0	0.055312	3.781813
1	0.833187	1.361453
2	1.299912	0.490123
3	1.579947	0.176444
4	1.747968	0.063520
5	1.848781	0.022867
6	1.909269	0.008232
7	1.945561	0.002964

Notice β_1 accelerates and then slows down. Why?



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-gradient-descent.ipynb>

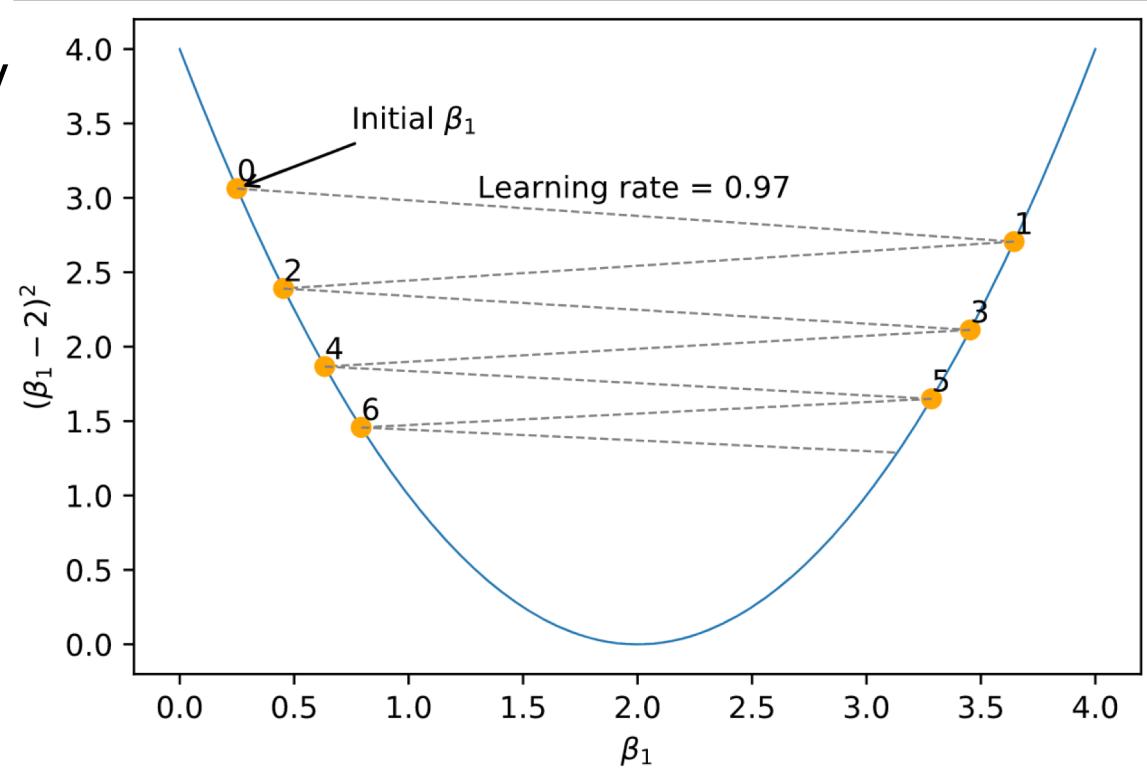
1D function minimization in action



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-gradient-descent.ipynb>

What if we crank up learning rate?

- β_1 oscillates across valley
- Picking learning rate is trial and error for our purposes but small like $\eta=.00001$ is a reasonable guess to start out
- If too small, we don't make progress to min

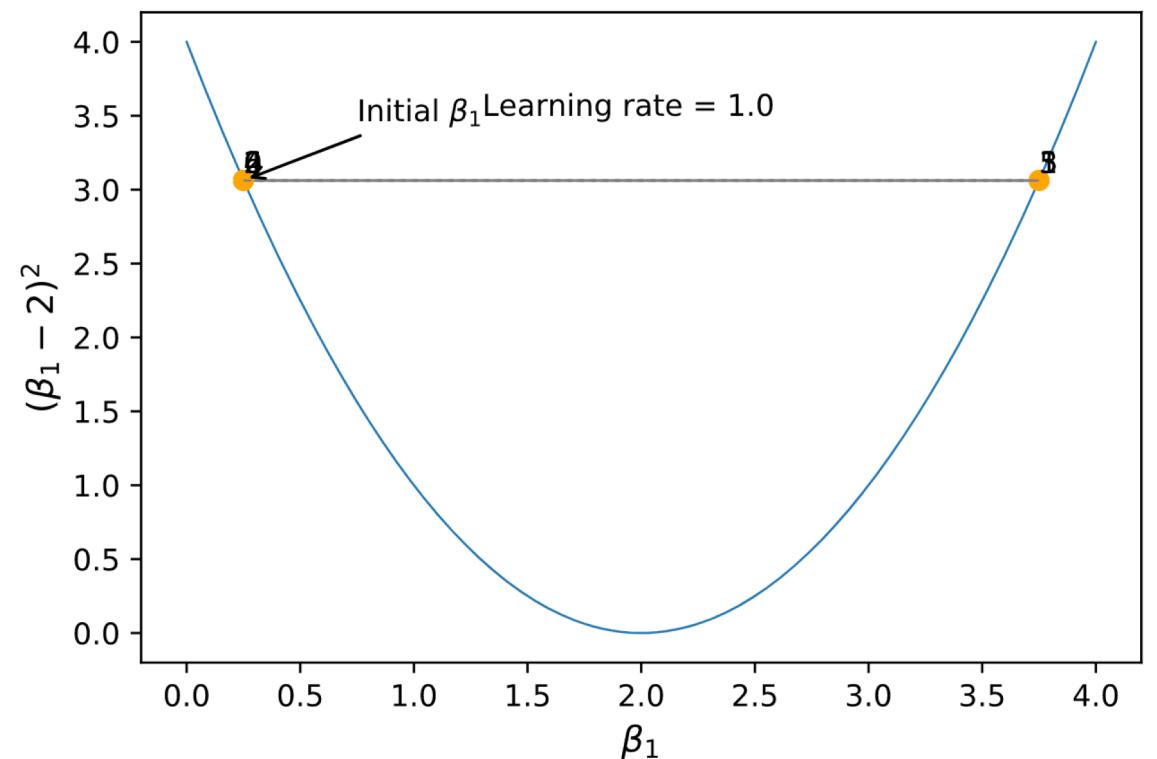


What if learning rate is really too high?

- We get nowhere:

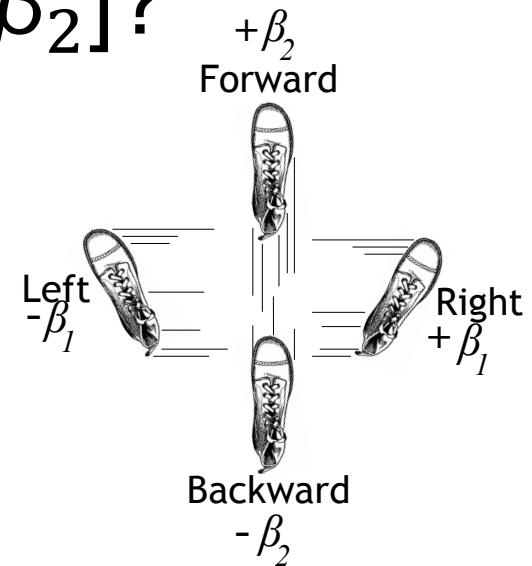
	beta_1	loss
0	0.495633	2.263119
1	3.504367	2.263119
2	0.495633	2.263119
3	3.504367	2.263119
4	0.495633	2.263119

- It can even diverge, exploding β_1

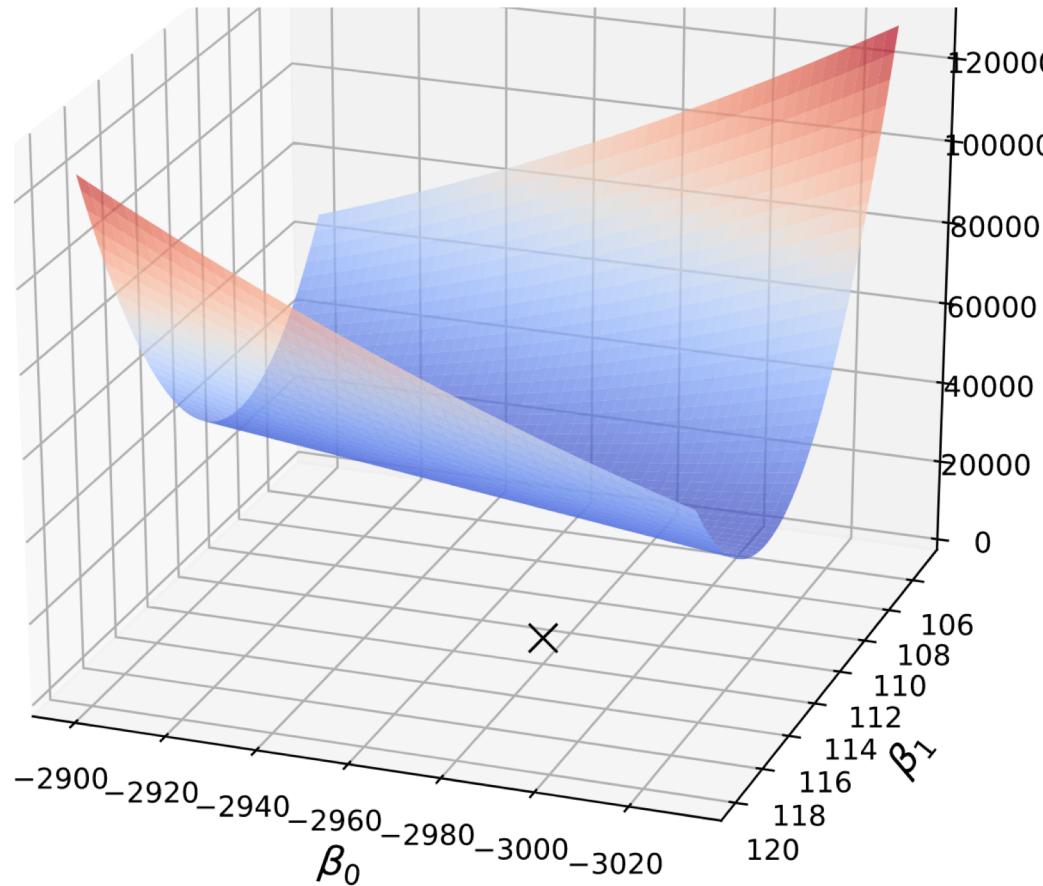


What happens in 2D for $\beta = [\beta_1, \beta_2]$?

- Imagine you're stuck on a mountain in the dark and need to get to the bottom
- Take steps to left, right, forward, backward or at an angle to minimize the “elevation function”
- Treat each direction separately, then combine into vector them to obtain the best step direction
- Each direction’s slope is a *partial derivative* and, combined, are the *gradient* vector



Loss function: 1-var regr. w/2 coeff (β_0, β_1)

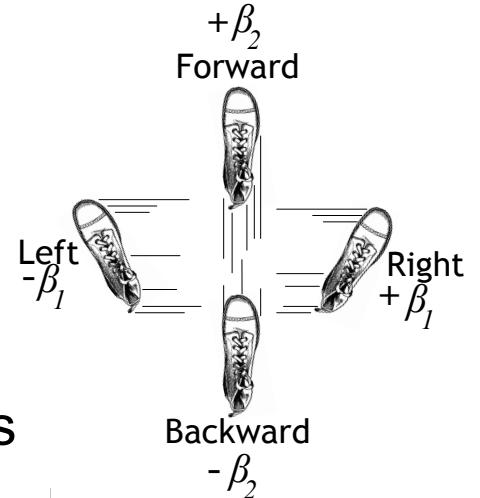


- Shallow in β_0 dir
- Steep in β_1 dir
- This plot show loss for non-standardized variables so a unit change in β_0 doesn't change loss nearly as much for β_1

Notation and finite difference approximation

- “Rise over run” is the derivative/slope of $f(x)$ at x :

$$\frac{d}{dx} f(x) = \frac{\partial}{\partial x} f(x) \approx \frac{f(x + h) - f(x)}{h}$$



- Gradient of $p > 1$ \mathbf{x} vector has p partial derivative entries

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{x_1} f(\mathbf{x}) \\ \frac{\partial}{x_2} f(\mathbf{x}) \end{bmatrix} \approx \begin{bmatrix} \frac{f([x_1+h, x_2]) - f(\mathbf{x})}{h} \\ \frac{f([x_1, x_2+h]) - f(\mathbf{x})}{h} \end{bmatrix}$$

- The partial derivative is just the slope in 1 dir, holding others constant

See <https://explained.ai/matrix-calculus/index.html>

General gradient descent

- Partial derivative is rate of change in one direction: $\frac{\partial}{\partial \beta_i} \mathcal{L}(\beta)$
- Combining partial derivatives into vector gives the *gradient*: ∇_{β}
- Gradient points in direction of increased loss, so must go in negative gradient direction to decrease loss as before:

$$\beta^{(t+1)} = \beta^{(t)} - \eta \nabla_{\beta} \mathcal{L}(\beta^{(t)}) \quad \text{where } \eta \text{ is a learning rate}$$

- Gradients have magnitude and direction
- E.g., gradient of $\beta=[-1, 2]$ means take step to left, but bigger step forward
- Take that single step: $\beta = \beta - \eta * [-1, 2]$
- In each direction, the partial derivative of loss function is 0 when flat
- When gradient vector = 0 vector, we're at min loss; choose that β

Update equation needs gradient:

$$\beta^{(t+1)} = \beta^{(t)} - \nabla_{\beta} \mathcal{L}(\beta^{(t)})$$

Gradient of $\mathcal{L}(\beta) = (\mathbf{y} - \mathbf{X}'\beta) \cdot (\mathbf{y} - \mathbf{X}'\beta)$ for lin regression is

$$\nabla_{\beta} \mathcal{L}(\beta) = -2\mathbf{X}'^T(\mathbf{y} - \mathbf{X}'\beta)$$

So update equation becomes (adding *learning rate* η):

$$\beta^{(t+1)} = \beta^{(t)} + \eta \mathbf{X}'^T(\mathbf{y} - \mathbf{X}'\beta^{(t)})$$

η scales the step we take each at each step (fold 2 into η)

Simplest gradient descent algorithm

Algorithm: *basic_minimize(\mathbf{X} , \mathbf{y} , \mathcal{L} , $\nabla\mathcal{L}$, η)* **returns** coefficients \vec{b}

Let $\vec{b} \sim 2N(0, 1) - 1$ (*init b with random $p + 1$ -sized vector with elements in $[-1, 1]$*)

$\mathbf{X}' = (\vec{1}, \mathbf{X})$ (*Add first column of 1s to data*) **except for L1/L2 regression**

repeat

$\vec{b} = \vec{b} - \eta \nabla \mathcal{L}$ **new direction**

until $|(\mathcal{L}(\vec{b}) - \mathcal{L}(\vec{b}_{prev}))| < precision;$

return \vec{b}

Adding momentum to particle update

- Reinforce movement in same direction; add fraction of previous dir

Algorithm: $\text{minimize}(\mathbf{X}, \mathbf{y}, \mathcal{L}, \nabla \mathcal{L}, \eta, \gamma)$ **returns** coefficients \vec{b}

Let $\vec{b} \sim 2N(0, 1) - 1$ (*random p + 1-sized vector with elements in [-1,1]*)

$\mathbf{X}' = (\vec{1}, \mathbf{X})$ (*Add first column of 1s*) **except for L1/L2 regression**

repeat

$$\vec{v} = \boxed{\gamma \vec{v}} + \boxed{\eta \nabla \mathcal{L}}$$

(*Add a bit of previous direction to next direction*)

$$\vec{b} = \vec{b} - \vec{v}$$

until $|(\mathcal{L}(\vec{b}) - \mathcal{L}(\vec{b}_{\text{prev}}))| < \text{precision};$

return \vec{b}

γ is a new hyper parameter

General Adagrad gradient descent

- Single learning rate for all dimensions is brutally slow
- Imagine long shallow valley with steep walls
- η small enough for steep walls is way too slow for other, shallow dimension

Algorithm: $adagrad_minimize(\mathbf{X}, \mathbf{y}, \mathcal{L}, \nabla \mathcal{L}, \eta, \epsilon=1e-5)$ returns coefficients \vec{b}

Let $\vec{b} \sim 2N(0, 1) - 1$ (*random p + 1-sized vector with elements in [-1, 1]*)

$h = \vec{0}$ (*p + 1-sized sum of squared gradient history*)

$\mathbf{X}' = (\vec{1}, \mathbf{X})$ (*Add first column of 1s*) **except for L1/L2 regression**

repeat

$\vec{h} += \nabla \mathcal{L} \otimes \nabla \mathcal{L}$ (*track sum of squared partials, use element-wise product*)

$\vec{b} = \vec{b} - \eta * \frac{\nabla \mathcal{L}}{(\sqrt{\vec{h}} + \epsilon)}$ **adjust w/update per β_i ; low h(istory) for β_i increases its learning rate**
(ϵ avoids divide by 0)

until $|(\mathcal{L}(\vec{b}) - \mathcal{L}(\vec{b}_{prev}))| < precision;$

return \vec{b}

See <http://cs231n.github.io/neural-networks-3/#ada>

Loss, gradient functions for minimization

- Linear regression

$$\mathcal{L}(\beta) = (\mathbf{y} - \mathbf{X}'\beta) \cdot (\mathbf{y} - \mathbf{X}'\beta)$$

$$\nabla_{\beta} \mathcal{L}(\beta) = -2\mathbf{X}'^T(\mathbf{y} - \mathbf{X}'\beta) \quad (\text{Can drop the 2, fold into learning rate})$$

- Logistic regression

$$\mathcal{L}(\beta) = \sum_{i=1}^n \left\{ y^{(i)} \mathbf{x}'^{(i)} \beta - \log(1 + e^{\mathbf{x}' \beta}) \right\}$$

$$\nabla_{\beta} \mathcal{L}(\beta) = -\mathbf{X}'^T(\mathbf{y} - \sigma(\mathbf{X}' \cdot \beta))$$

L1, L2 regression loss, gradient functions

- L2 (Ridge); 0-center x_i then $\beta_0 = \text{mean}(\mathbf{y})$, find $\beta_{1..p}$ via:

$$\mathcal{L}(\beta) = (\mathbf{y} - \mathbf{X}\beta) \cdot (\mathbf{y} - \mathbf{X}\beta) + \lambda\beta \cdot \beta$$

$$\nabla_{\beta} \mathcal{L}(\beta) = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) + 2\lambda\beta \quad (\text{Can drop the } 2, \text{ fold into learning rate})$$

- L1 (Lasso); 0-center x_i then $\beta_0 = \text{mean}(\mathbf{y})$, find $\beta_{1..p}$ via:

$$\mathcal{L}(\beta) = (\mathbf{y} - \mathbf{X}\beta) \cdot (\mathbf{y} - \mathbf{X}\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

$$\nabla_{\beta} \mathcal{L}(\beta) = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) + \lambda \text{sign}(\beta)$$

L1 logistic loss, gradient functions

- Must compute β_0 differently; partial β_0 is a function of β_0

$$\frac{\partial}{\partial \beta_0} \mathcal{L}(\beta, \lambda) = \text{mean}(\mathbf{y} - \sigma(\mathbf{X}' \cdot \beta))$$

- Other β_i are functions of β_0 but not within the penalty term

$$\nabla_{\beta_{1..p}} \mathcal{L}(\beta, \lambda) = \frac{1}{n} \left\{ \mathbf{X}^T (\mathbf{y} - \sigma(\mathbf{X}' \cdot \beta')) - \lambda \text{sign}(\beta) \right\}$$

- Combine to get full gradient vector

L1 logistic gradient algorithm

(review from regularization lecture)

Algorithm: $L1NegLogLikelihood(\mathbf{X}', \mathbf{y}, \beta')$

$err = \mathbf{y} - \sigma(\mathbf{X}' \cdot \beta')$ (error vector is $n \times 1$ column vector)

$\frac{\partial}{\partial \beta_0} = mean(err)$ (usual log-likelihood gradient; use current β')

$r = \lambda \text{sign}(\beta')$ (regularization term $p + 1 \times 1$ column vector)

$r[0] = 0$ (kill β_0 position but keep as $p + 1 \times 1$ vector)

$\nabla = \frac{1}{n} \{ \mathbf{X}'^T err - r \}$

return –
$$\begin{bmatrix} \frac{\partial}{\partial \beta_0} \\ \nabla_1 \\ \vdots \\ \nabla_p \end{bmatrix}$$

Key takeaways

- Move towards lower loss; consider each direction separately
- Slope in direction β_i is partial derivative: $\frac{\partial}{\partial \beta_i} \mathcal{L}(\beta)$
- Gradient is p or $p+1$ dimensional vector of partial derivatives
- Gradients point “upwards” towards higher cost/loss
- Coefficients should therefore move in opposite direction of gradient
- Gradient is the 0 vector at the minimum loss; i.e., flat
- Can stop optimizing when gradient is close to 0 vector or when $\beta_i^{(t+1)}$ is very close to $\beta_i^{(t)}$ or after fixed number of iterations

More key takeaways

- Coefficient update equation:

$$\beta^{(t+1)} = \beta^{(t)} - \eta \nabla_{\beta} \mathcal{L}(\beta^{(t)}) \quad \text{where } \eta \text{ is a learning rate}$$

- If η is “small enough,” $\beta_i^{(t+1)}$ will converge to a solution vector (maybe slowly)
- If too big, will bounce back and forth across valleys or diverge
- Adagrad
 - Single learning rate too slow; need a rate per dimension
 - Increases update step size for dimensions with shallow slopes historically
 - Slows down across all dimensions over time as history sum h gets bigger
- L1, L2 linear regression doesn’t optimize β_0 , it’s just mean(\mathbf{y}), if we 0-center x_i
- L1, L2 logistic regression optimizes $\beta_{0..p}$ but β_0 differently than $\beta_{1..p}$

Lab time

- Exploring regularization for linear regression
<https://nbviewer.jupyter.org/github/parrt/msds621/blob/master/labs/linear-models/gradient-descent.ipynb>
- Note: that link is for viewing since github screws that up; you will need to go to the course repo to get interactive labs
<https://github.com/parrt/msds621/tree/master/labs/linear-models>