Stochastic Gradient Descent Part I

Linear Regression

Previously on CSCI 4622

Given data $(x_{i1}, x_{i2}, \ldots, x_{ip}, y_i)$ for $i = 1, 2, \ldots, n$ fit a MLR model of the form

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \epsilon_i \qquad \text{where} \qquad \epsilon_i \sim N(0, \sigma^2)$$

by minimizing $$\mathrm{RSS}_\lambda = \sum_{i=1}^{n} \left[(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i\right]^2 + \lambda \sum_{k=1}^{p} \beta_k^2$$

Given data $(x_{i1}, x_{i2}, \ldots, x_{ip}, y_i)$ for $i = 1, 2, \ldots, n$ fit a LogReg model of the form

$$p(y = 1 \mid x) = \mathrm{sigm}(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)$$

as we'll see later this week, by minimizing a similar loss function.

Finding Parameters in Linear Regression

Whether doing simple linear regression or multiple linear regression, parameters are estimated by minimizing the RSS loss function.

$$\mathrm{RSS}_\lambda = \sum_{i=1}^{n} [(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i]^2 + \lambda \sum_{k=1}^{p} \beta_k^2$$

When you lots of data and a model with many features, this becomes a difficult problem

While direct methods (based on linear algebra) exist, they are far too memory and computationally expensive to perform in real life

Instead, we use an **iterative method**

Iterative Solution Methods

Iterative methods can be thought of as very intelligent guess and check

$$y_i = \beta_0 + \beta_1 x_i$$

- Make a guess at the parameters
- Update your guess in a smart way, based on the problem specs, to get a better guess
- Repeat until guess converges to something very close to the correct answer

$$\beta_0^{(0)} \to \beta_0^{(1)} \to \cdots \to \beta_0^{(k)} \approx \beta_0$$

$$\beta_1^{(0)} \to \beta_1^{(1)} \to \cdots \to \beta_1^{(k)} \approx \beta_1$$

A Silly Example

Suppose you want to find the minimum of the function $f(z) = z^2 - 2z + 2$

We can rewrite in a slightly better form:

minimizer is $z=1$

$$f(z) = (z-1)^2 + 1$$

Question: What nice properties for minimization does this function have?

A Silly Example

Suppose you want to find the minimum of the function $f(z) = z^2 - 2z + 2$

OK, suppose that I guess that the minimizer is $z^{(0)} = 2.25$

Question: Which way should I move?

$f'(z) = 2z - 2$

$f'(2.25) =$

$2 \cdot 2.25 - 2$

$= 2.5$

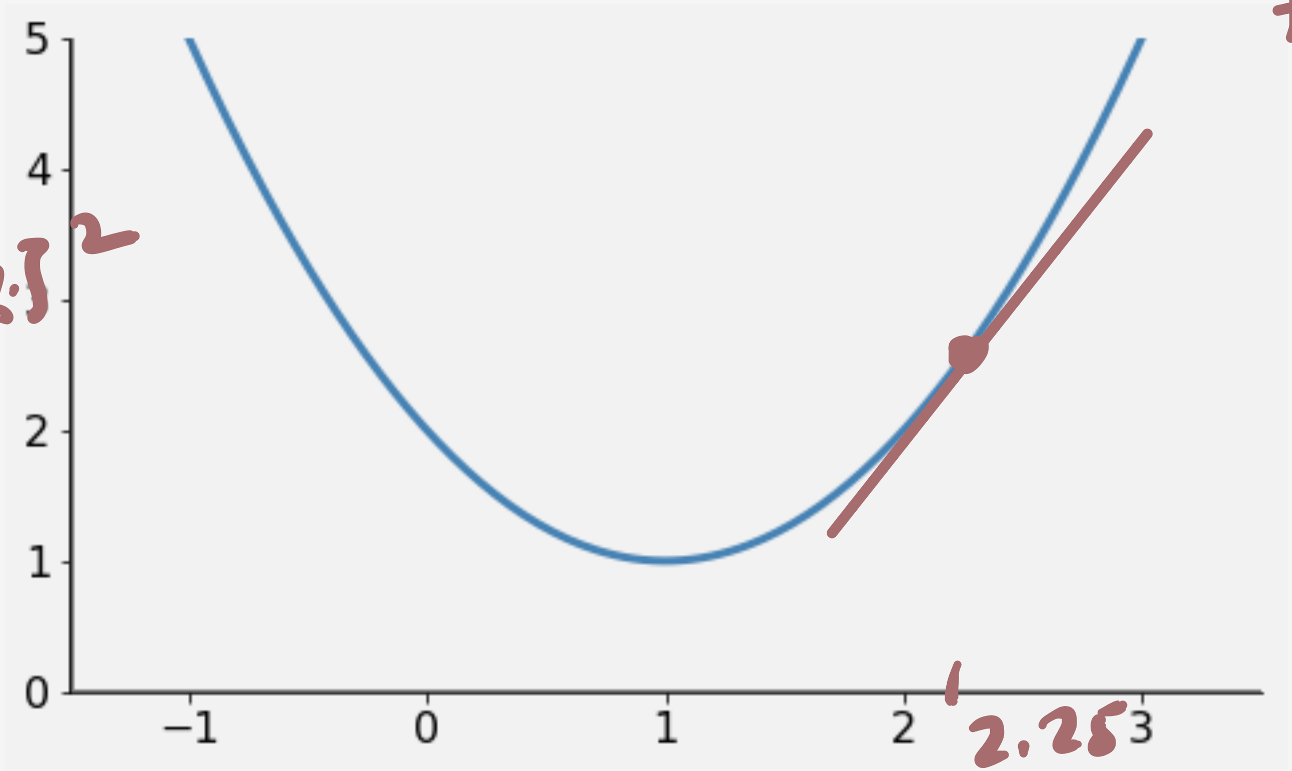
f' is > 0

move LEFT

$f' < 0$

$\rightarrow$ move RIGHT

RSS $= \sum_{i=1}^{n} [(\beta_0 + \beta_1 x_i) - y_i]^2$



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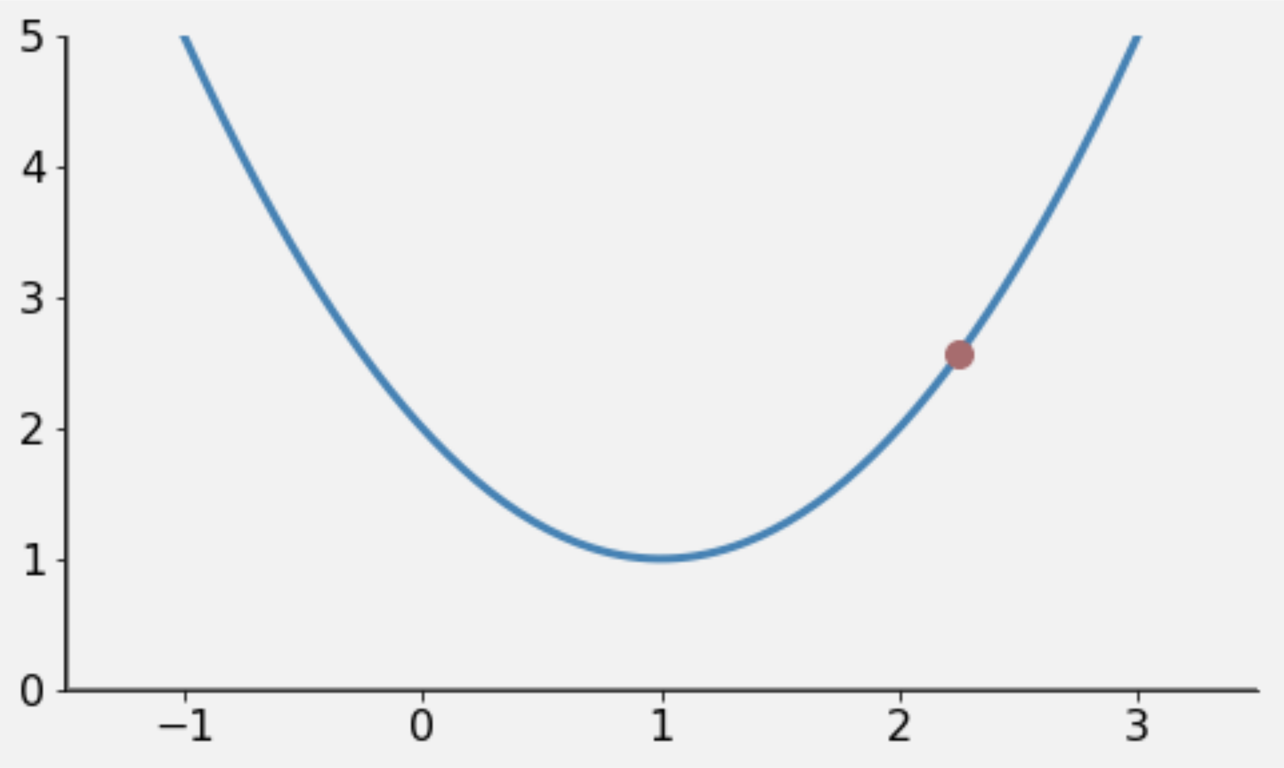
OK, suppose that I guess that the minimizer is $z^{(0)} = 2.25$

Question: Which way should I move? **Answer**: Downhill! But which way is down?



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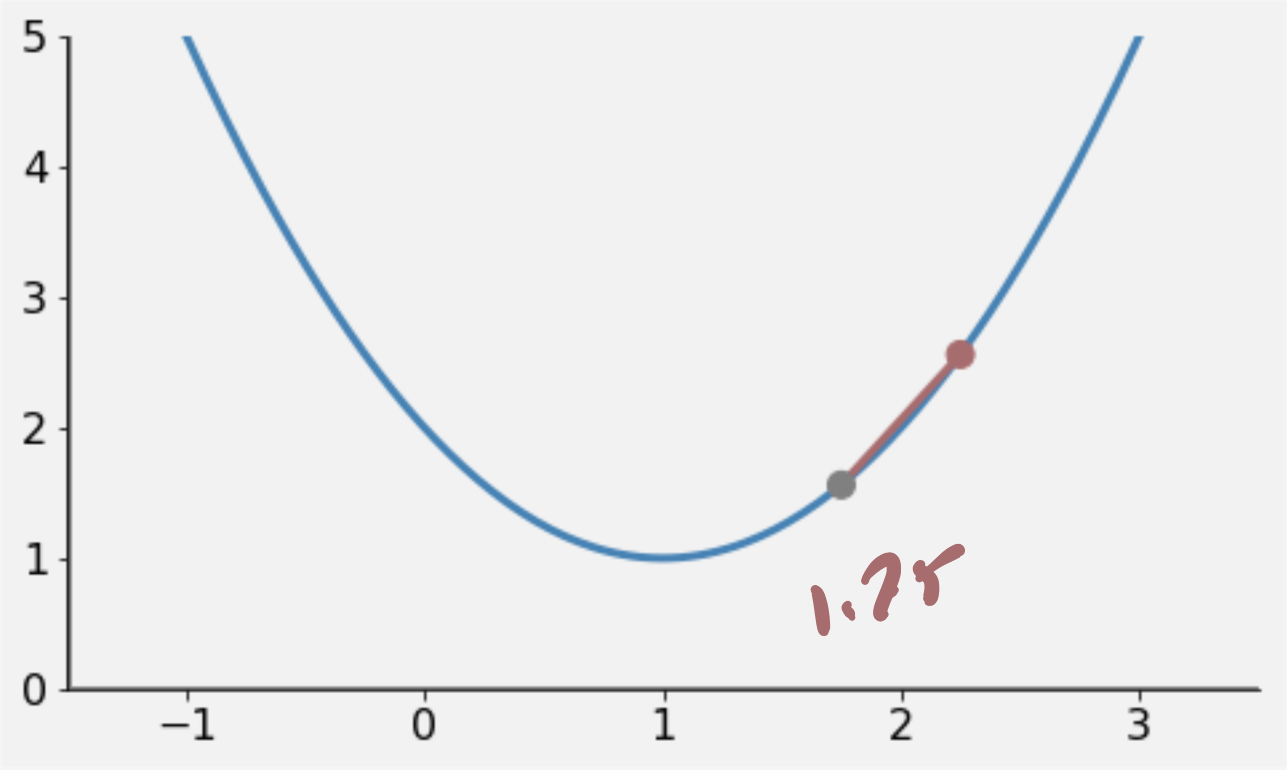

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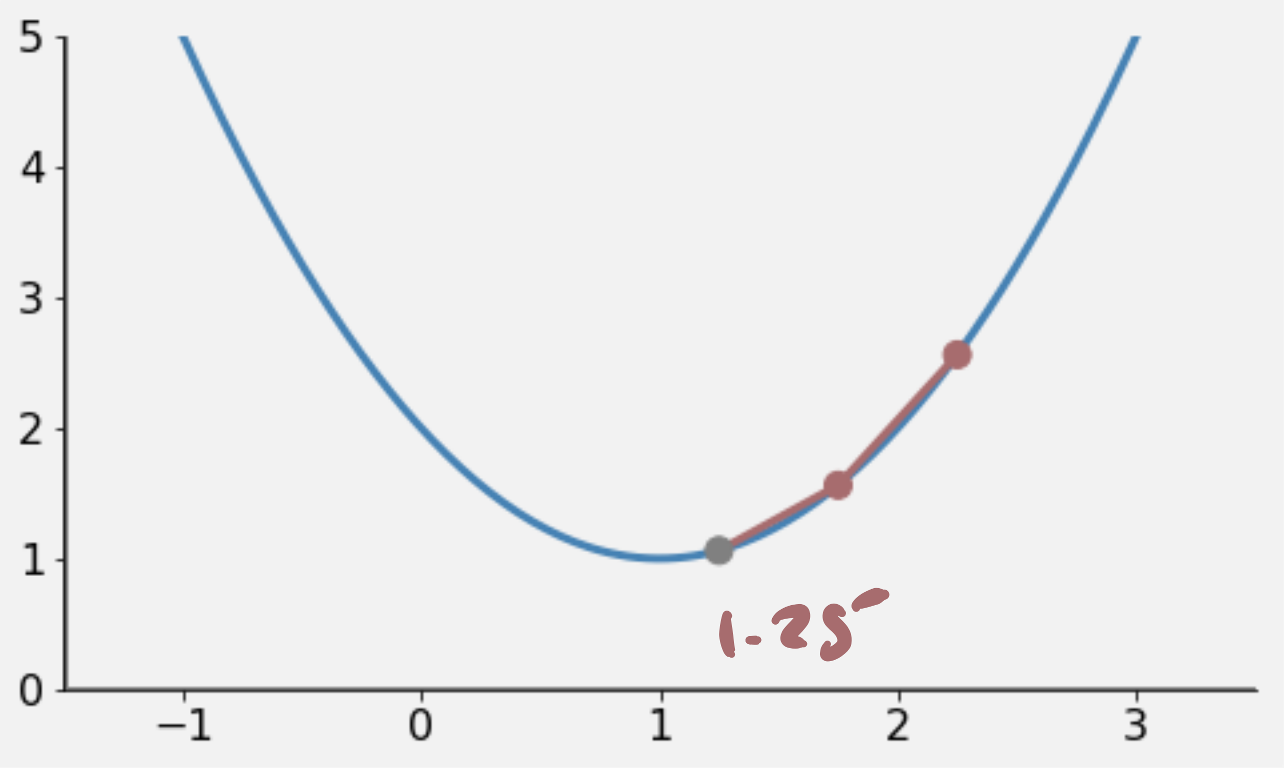

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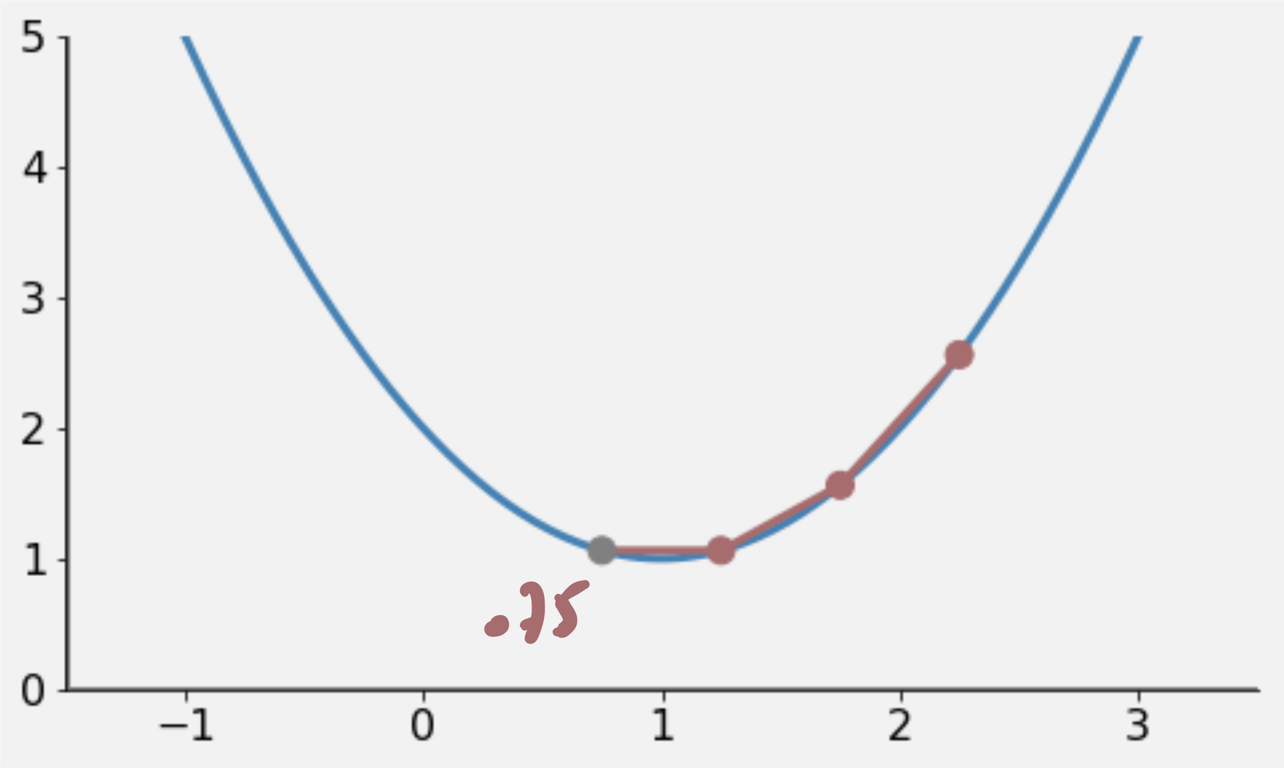

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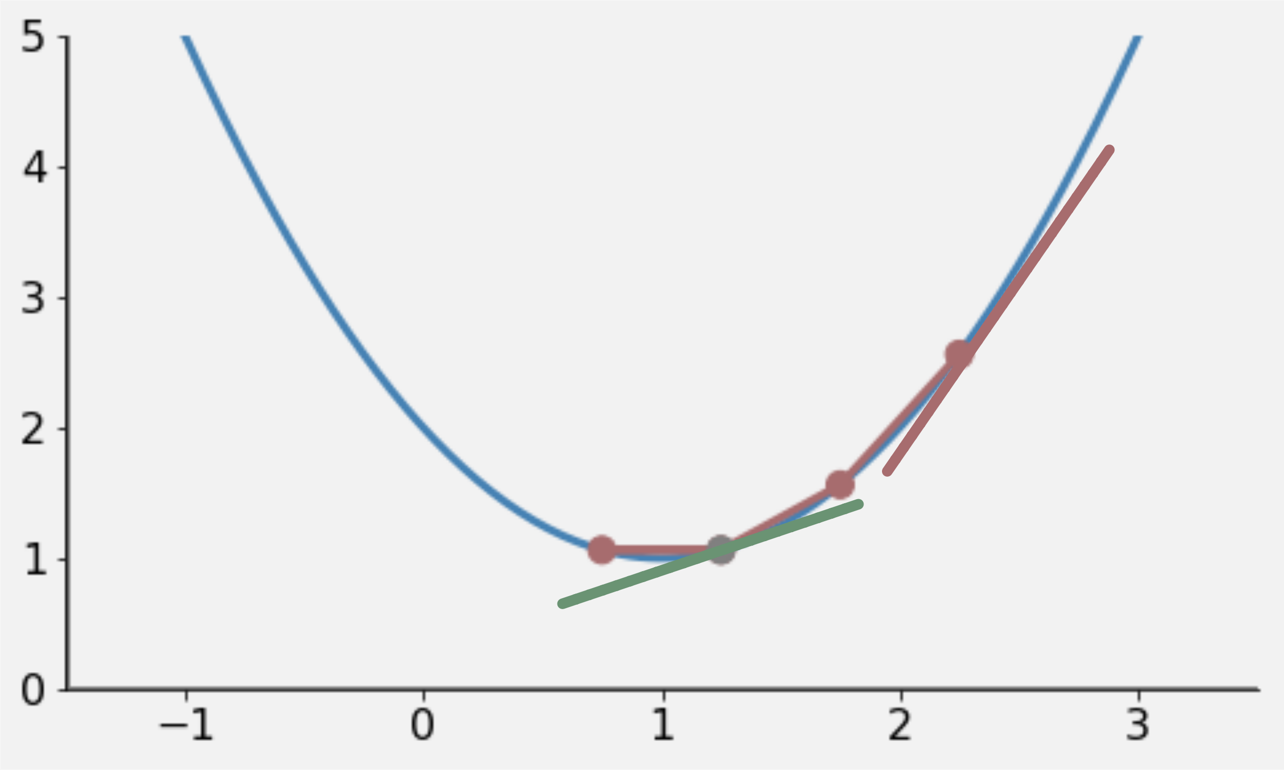
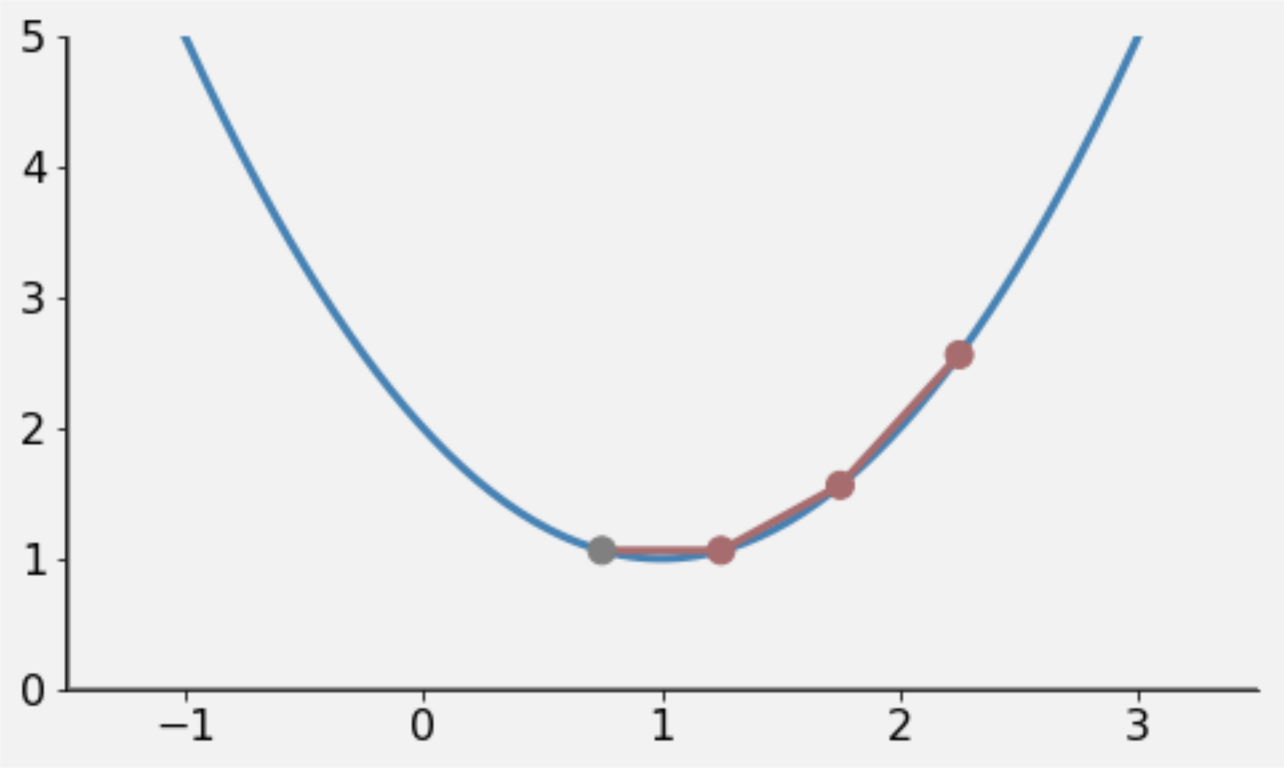


A Silly Example

Question: How do we fix this so we can get closer to the true minimum?

- BAD IDEA: REDUCE LEARNING RATE
- GOOD IDEA: MAKE STEP PROP to DERIV. SIZE

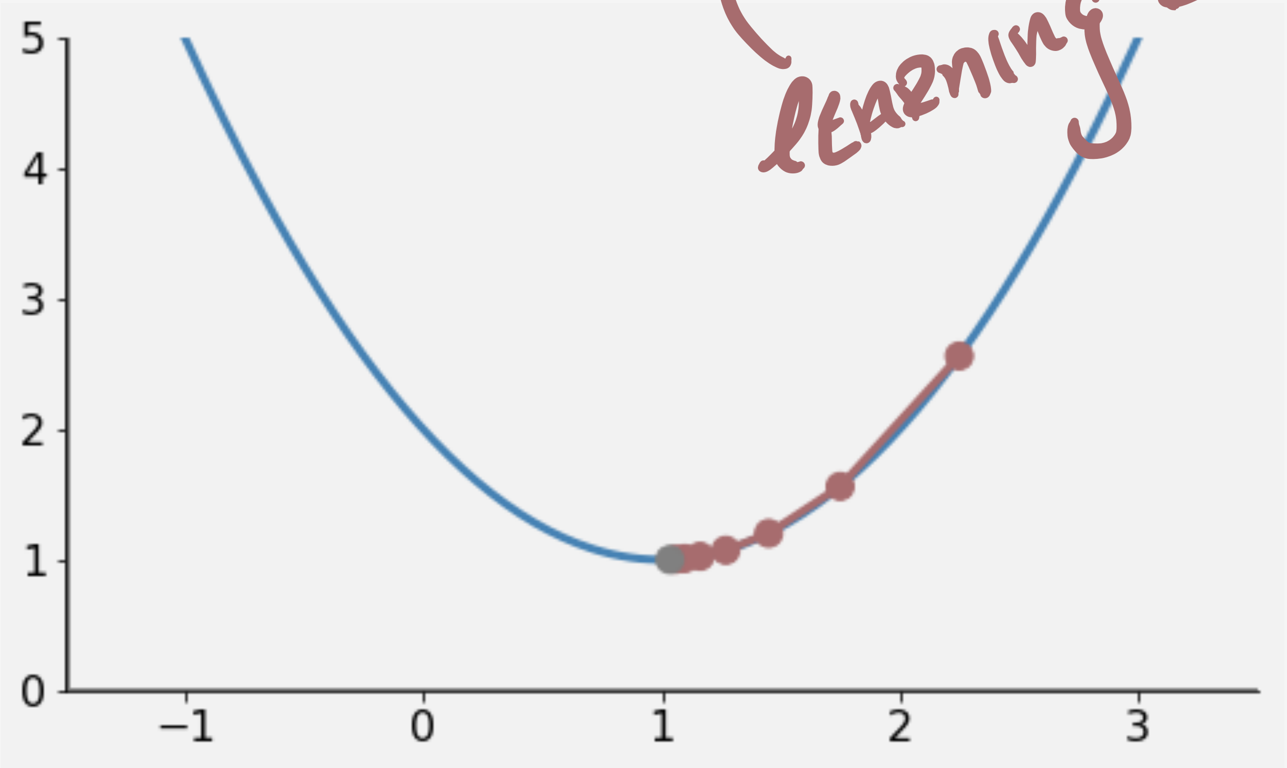


A Silly Example

This method is called **Gradient Descent** (think Derivative Descent)

$$z^{(k+1)} = z^{(k)} - \eta \cdot f'(z^{(k)})$$

LEARNING RATE



Simple Linear Regression

OK, so how do we use the idea of Gradient Descent to estimate the parameters in SLR

Recall, the estimated parameters are the value of β_0 and β_1 that minimize the RSS

$$\text{RSS} = \sum_{i=1}^{n} \left[(\beta_0 + \beta_1 x_i) - y_i\right]^2$$

Important: We're minimizing over the β's . The x's and y's are the values from the data.

The difficulty is that this is a function of two variables, which is not quite a simple parabola

Simple Linear Regression

In 1-dimension the RSS is a parabola. In 2-dimensions it's a bowl-like surface

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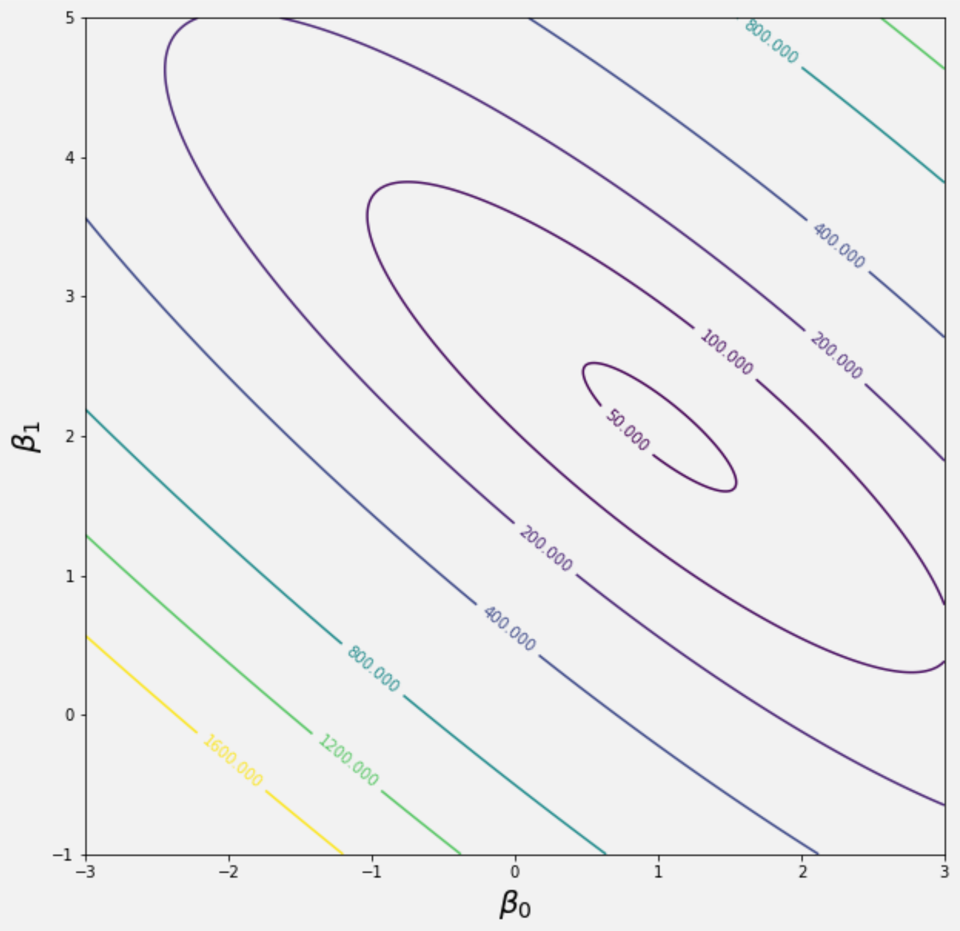

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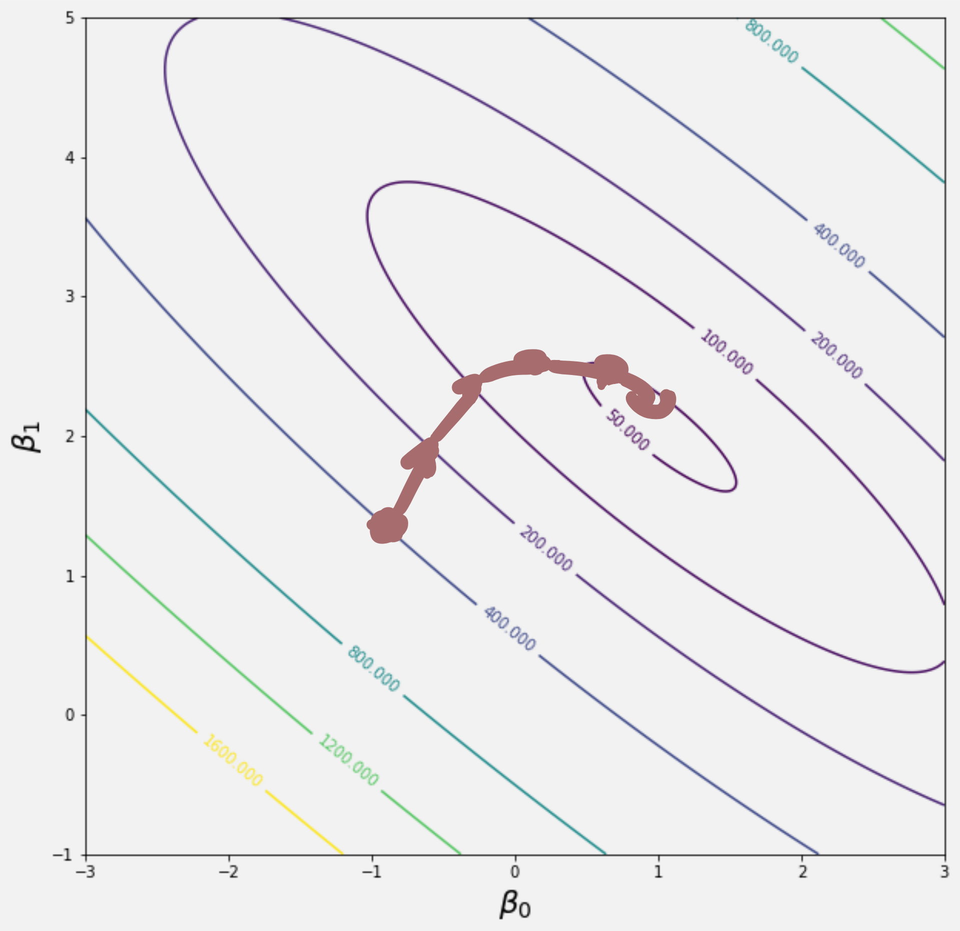
In 2D the process is still the same:

- Make a guess at the minimum
- Move iteratively downhill



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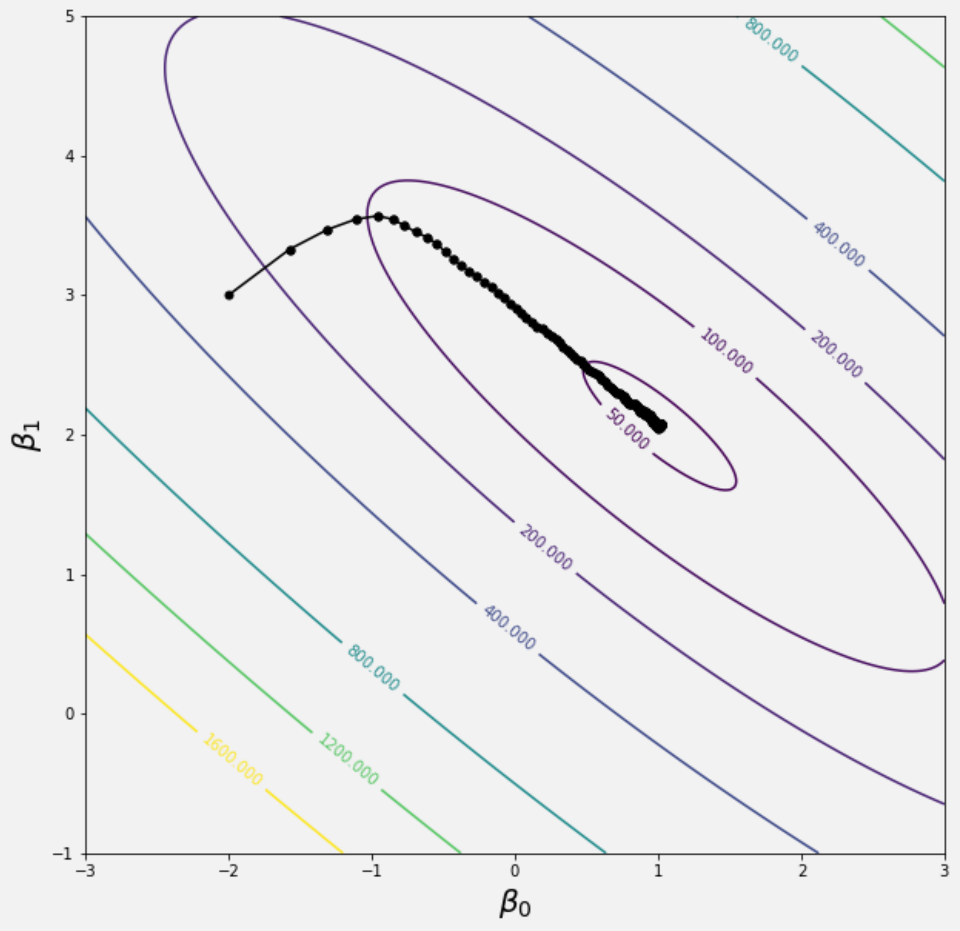

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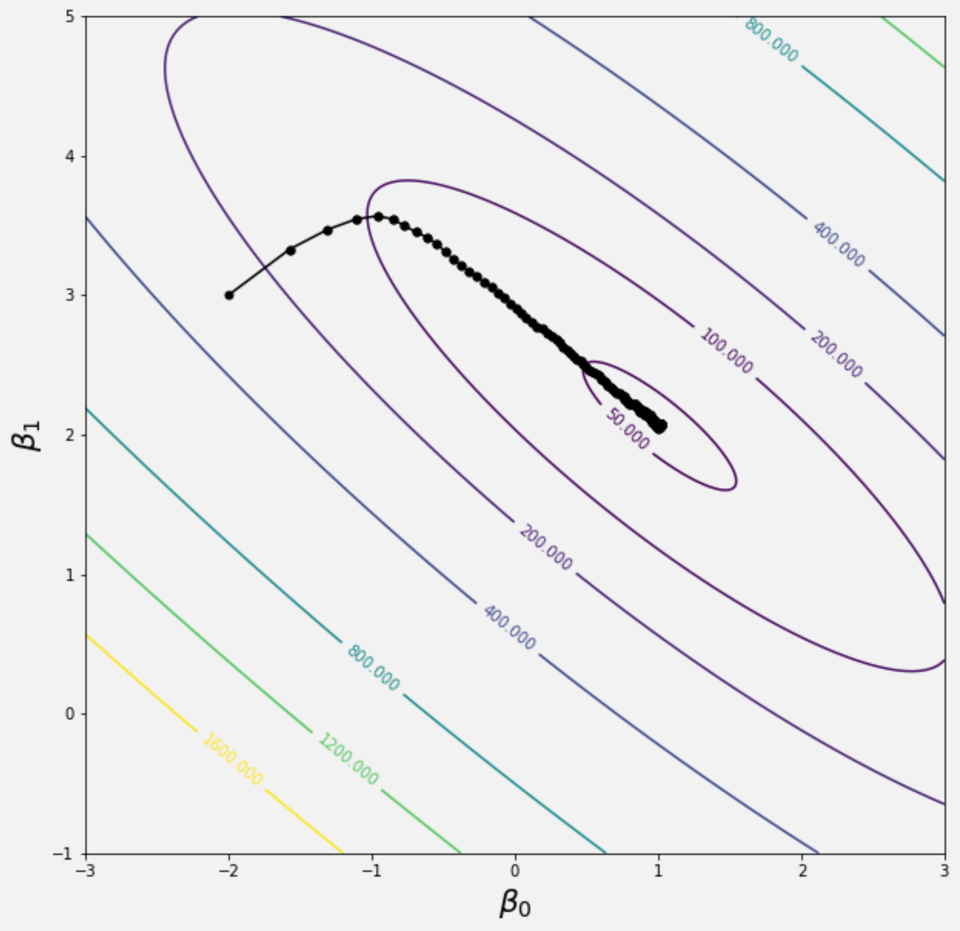
But how do we move downhill in 2d?



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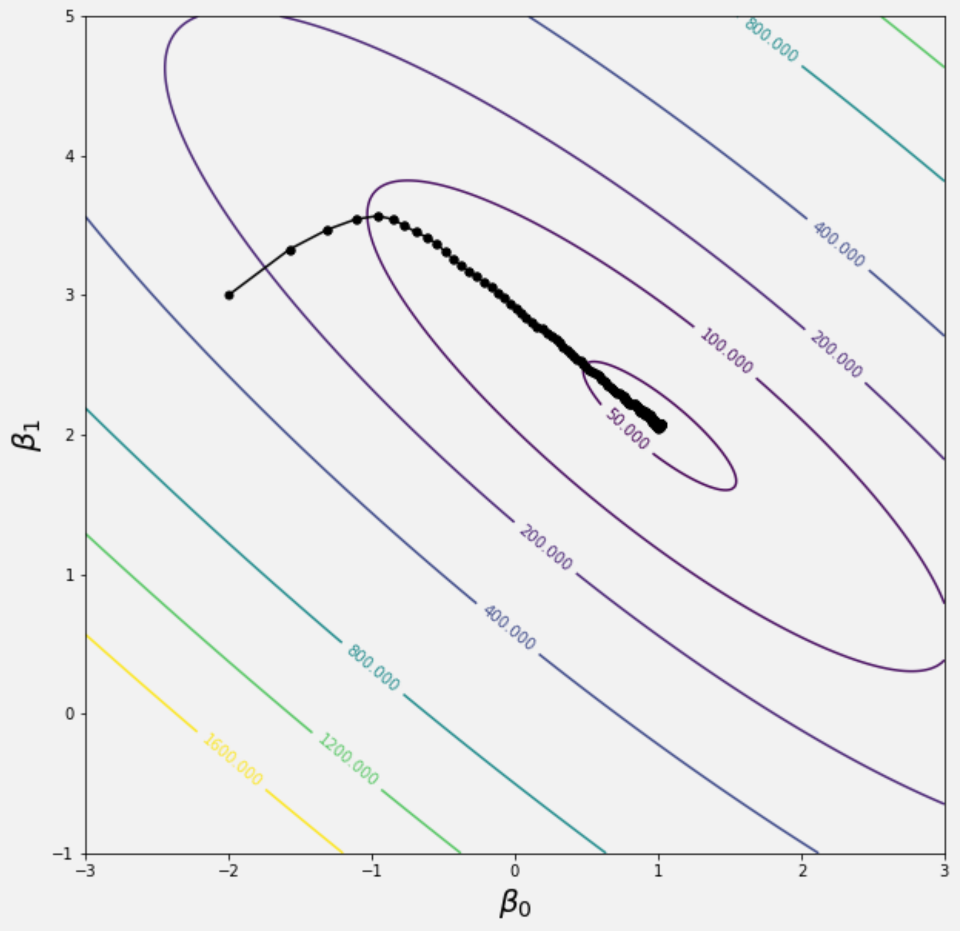

But how do we move downhill in 2d?

- Move downhill in each coordinate direction
- Use partial derivatives

Gradient Descent for SLR

In 1-dimension, Gradient Descent was $z^{(k+1)} = z^{(k)} - \eta \cdot f'(z^{(k)})$

In 2-dimensions, we have the following:

$$\beta_0 \quad \leftarrow \quad \beta_0 - \eta \frac{\partial \mathrm{RSS}}{\partial \beta_0}$$

$$\beta_1 \quad \leftarrow \quad \beta_1 - \eta \frac{\partial \mathrm{RSS}}{\partial \beta_1}$$

$$RSS = \sum_{i=1}^{n} [(\beta_0 + \beta_1 x_i) - y_i]^2$$

$$\frac{\partial RSS}{\partial \beta_0} = \sum_{i=1}^{n} 2[(\beta_0 + \beta_1 x_i) - y_i] \cdot 1$$

$$\frac{\partial RSS}{\partial \beta_1} = \sum_{i=1}^{n} 2[(\beta_0 + \beta_1 x_i) - y_i] x_i$$

Gradient Descent for SLR

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In 2-dimensions, we have the following:

$$\beta_0 \quad \leftarrow \quad \beta_0 - \eta \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right]$$

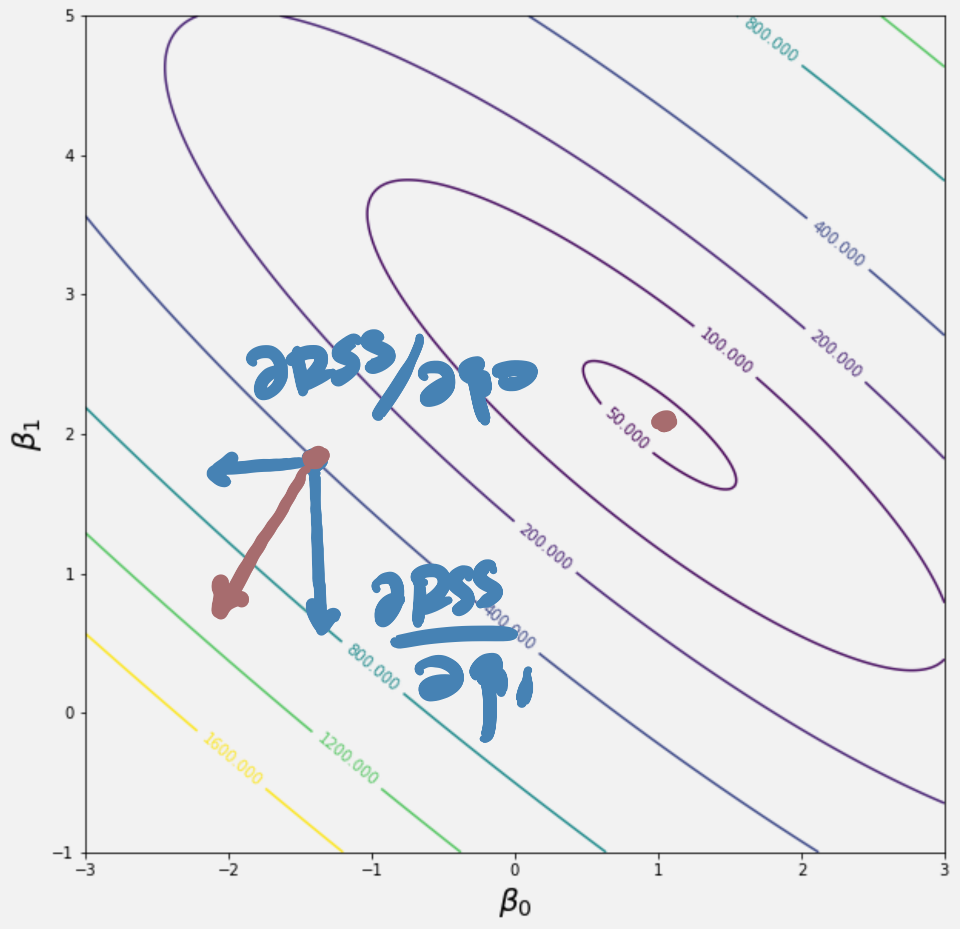
$$\beta_1 \quad \leftarrow \quad \beta_1 - \eta \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] x_i$$

Vectorizing Gradient Descent

Let $\boldsymbol{\beta} = [\beta_0, \beta_1]^T$ be vector of the parameters. Need to **vectorize** derivatives too

$$\frac{\partial \text{RSS}}{\partial \beta_0} = \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right]$$

$$\frac{\partial \text{RSS}}{\partial \beta_1} = \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] x_i$$



Vector of derivatives is called the **Gradient**

Points in direction that loss function increases the **fastest** (i.e. steepest direction)

Vectorizing Gradient Descent

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$$\nabla \mathrm{RSS} = \begin{bmatrix} \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] \\ \sum_{i=1}^{n} 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] x_i \end{bmatrix}$$

$$\boxed{\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \eta \nabla \mathrm{RSS}}$$

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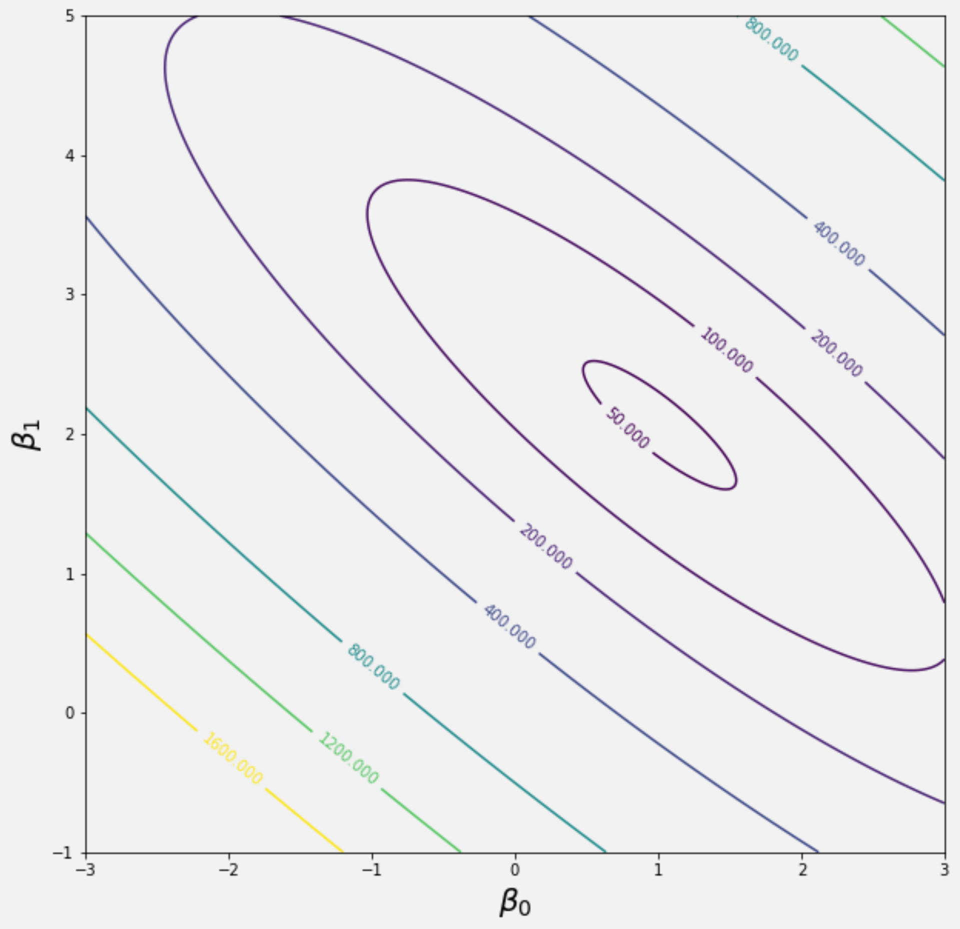


Vectorized Gradient Descent for SLR

OK, so we guess values of the parameters, and then perform gradient updates to improve

$$\begin{bmatrix} \beta_0 \\ \\ \beta_1 \end{bmatrix} \leftarrow \begin{bmatrix} \beta_0 \\ \\ \beta_1 \end{bmatrix} - \eta \begin{bmatrix} \sum_{i=1}^n 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] \\ \\ \sum_{i=1}^n 2\left[(\beta_0 + \beta_1 x_i) - y_i\right] x_i \end{bmatrix}$$

Question: Does anything about this seem slow?

Stochastic Gradient Descent

Update based on one training example at a time. Faster, but less accurate updates

FOR ONE TRAINING EX (x_i, y_i)

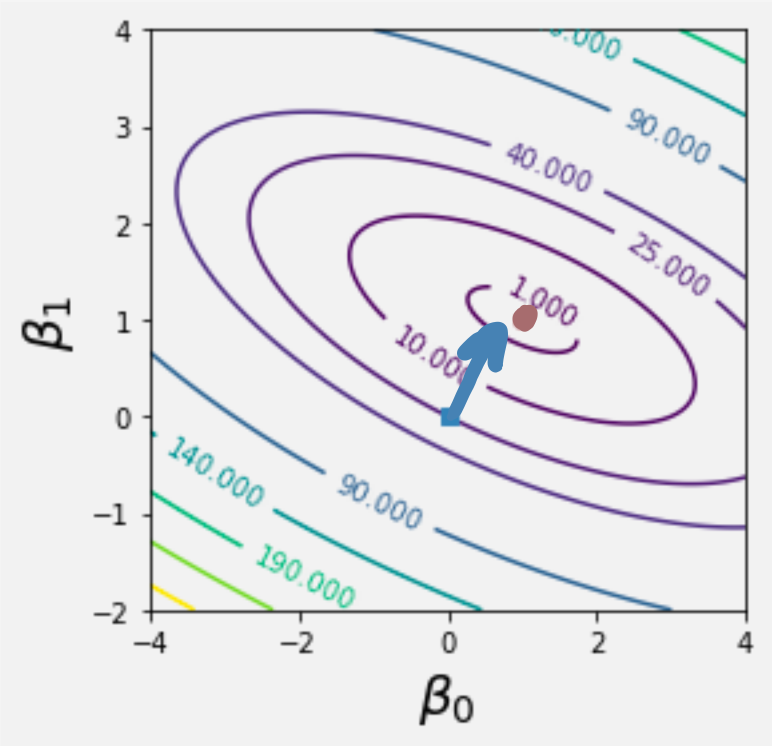
$$\begin{bmatrix} \beta_0 \\ \\ \beta_1 \end{bmatrix} \leftarrow \begin{bmatrix} \beta_0 \\ \\ \beta_1 \end{bmatrix} - \eta \begin{bmatrix} 2\left((\beta_0 + \beta_1 x_i) - y_i\right) \\ \\ 2\left((\beta_0 + \beta_1 x_i) - y_i\right) x_i \end{bmatrix}$$

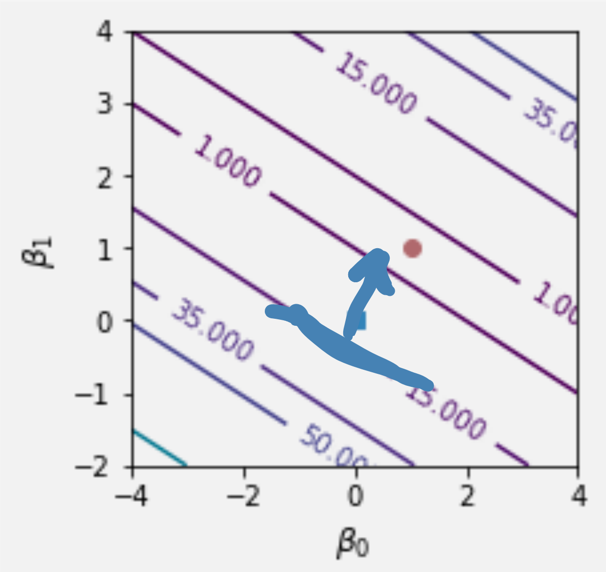
Important: Just like when training a Perceptron:

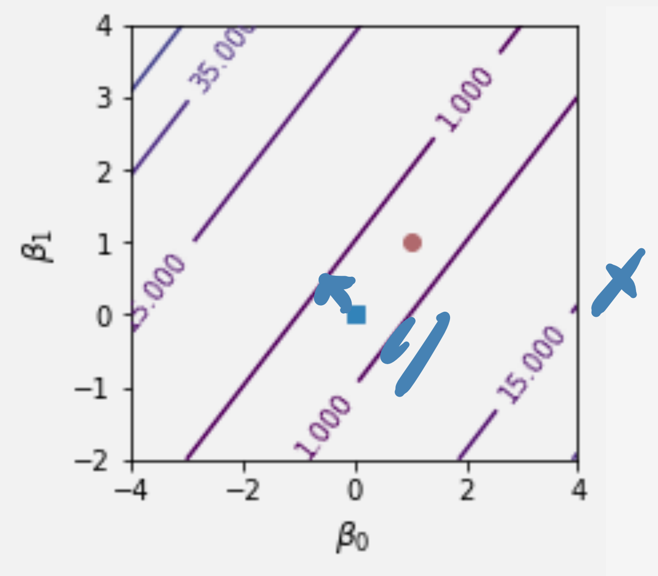
- Loop through training examples in random order to avoid bias
- Go through all training examples before starting over
- One pass through training examples is called an **Epoch**

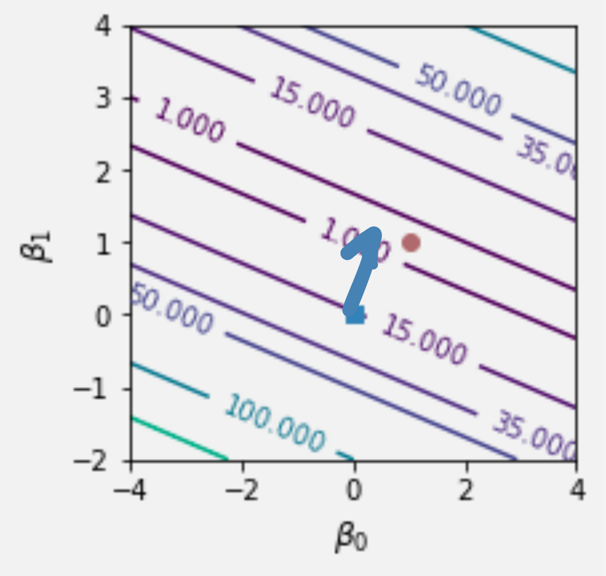
Geometry of Stochastic Gradient Descent

$$RSS_i = [(\beta_0 + \beta_1 x_i) - y_i]^2$$



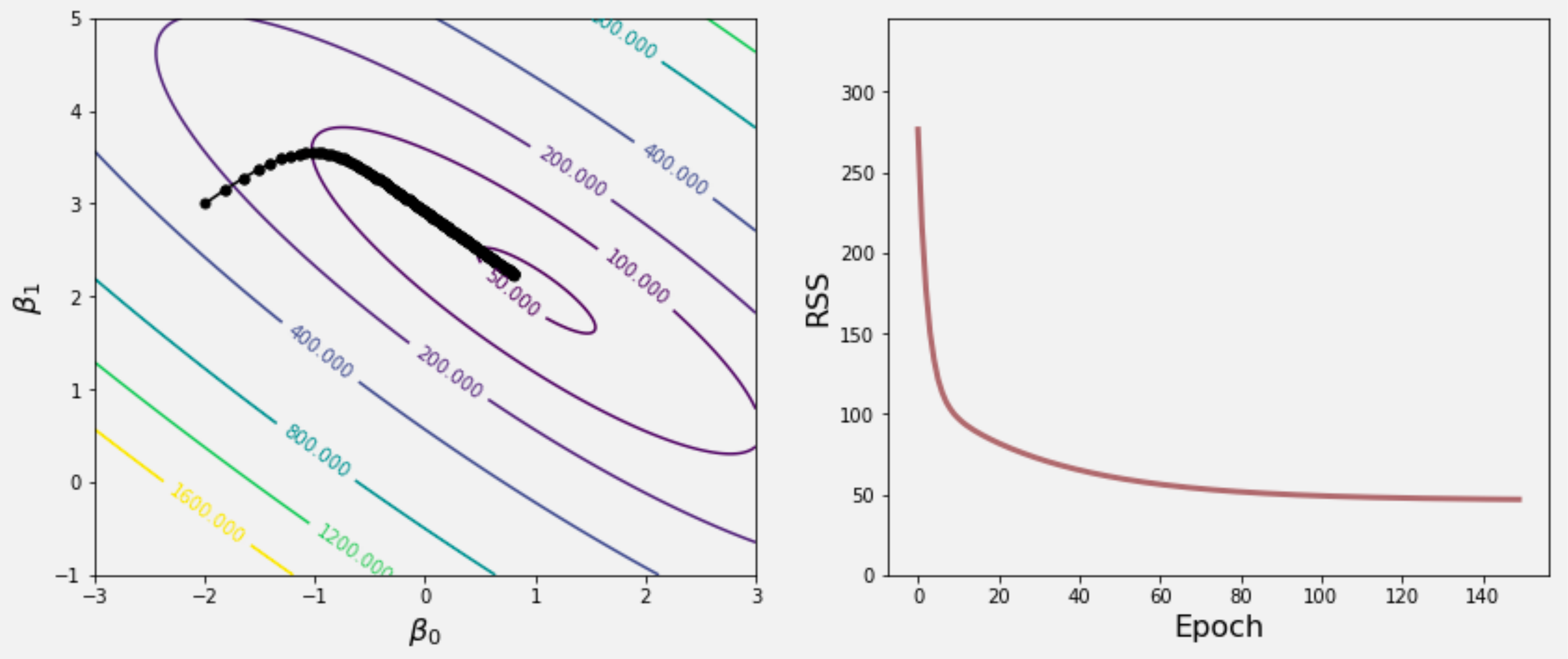






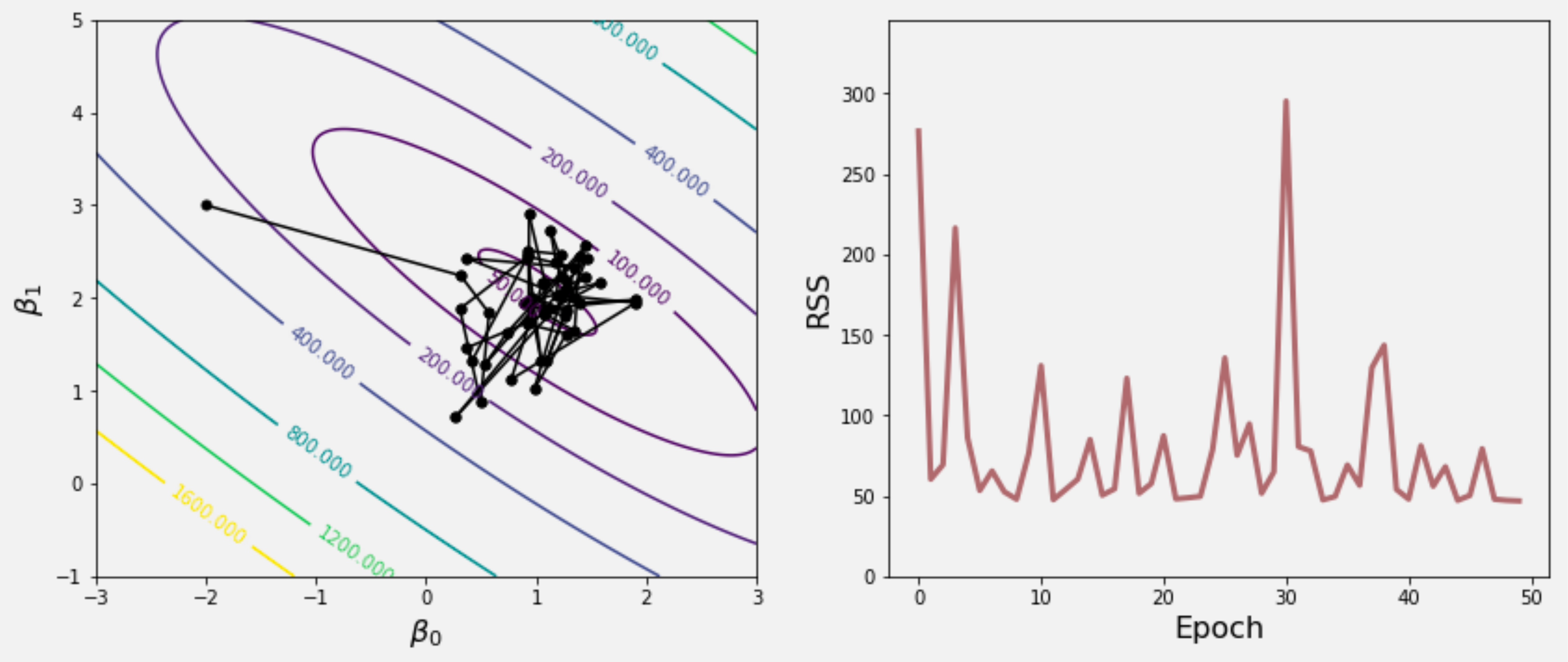
The Importance of the Learning Rate

Too small of a learning rate and it takes forever to converge



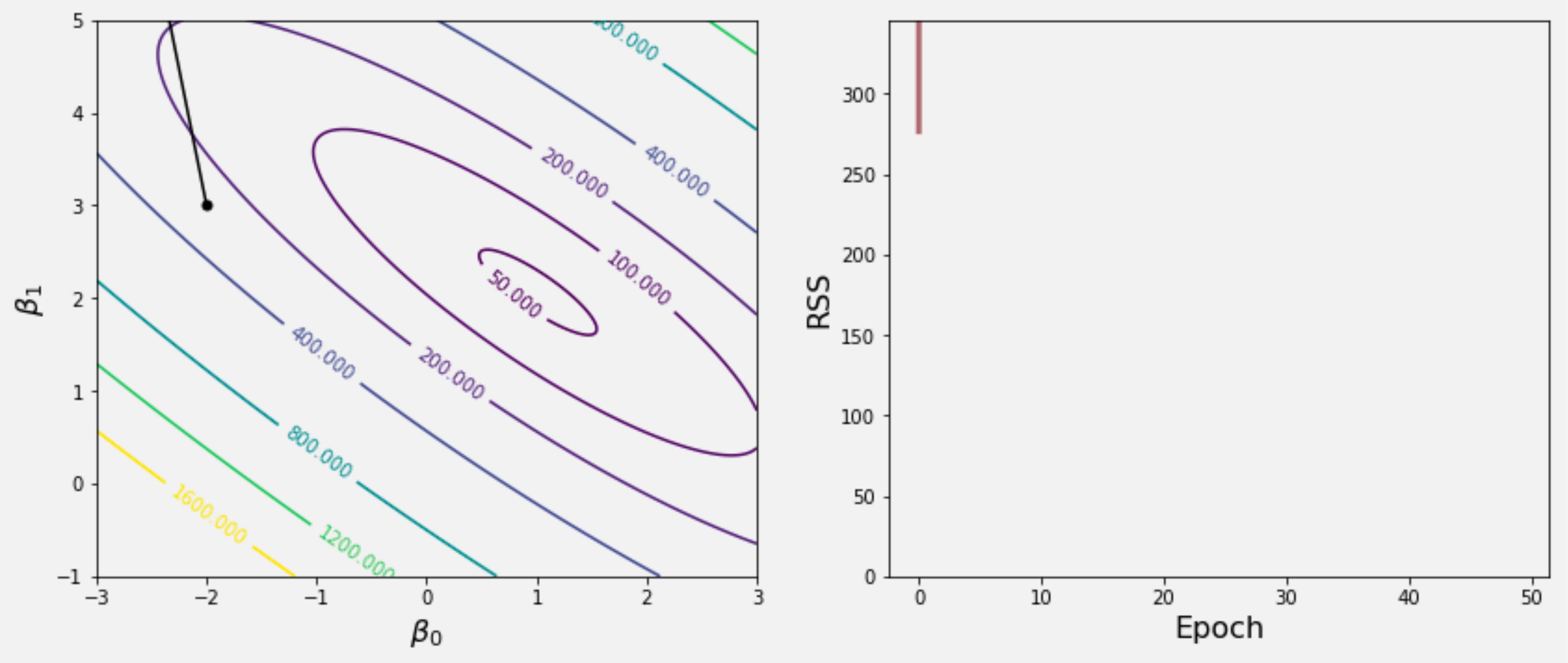
The Importance of the Learning Rate

Too large a learning rate and you can get oscillations that bounce around



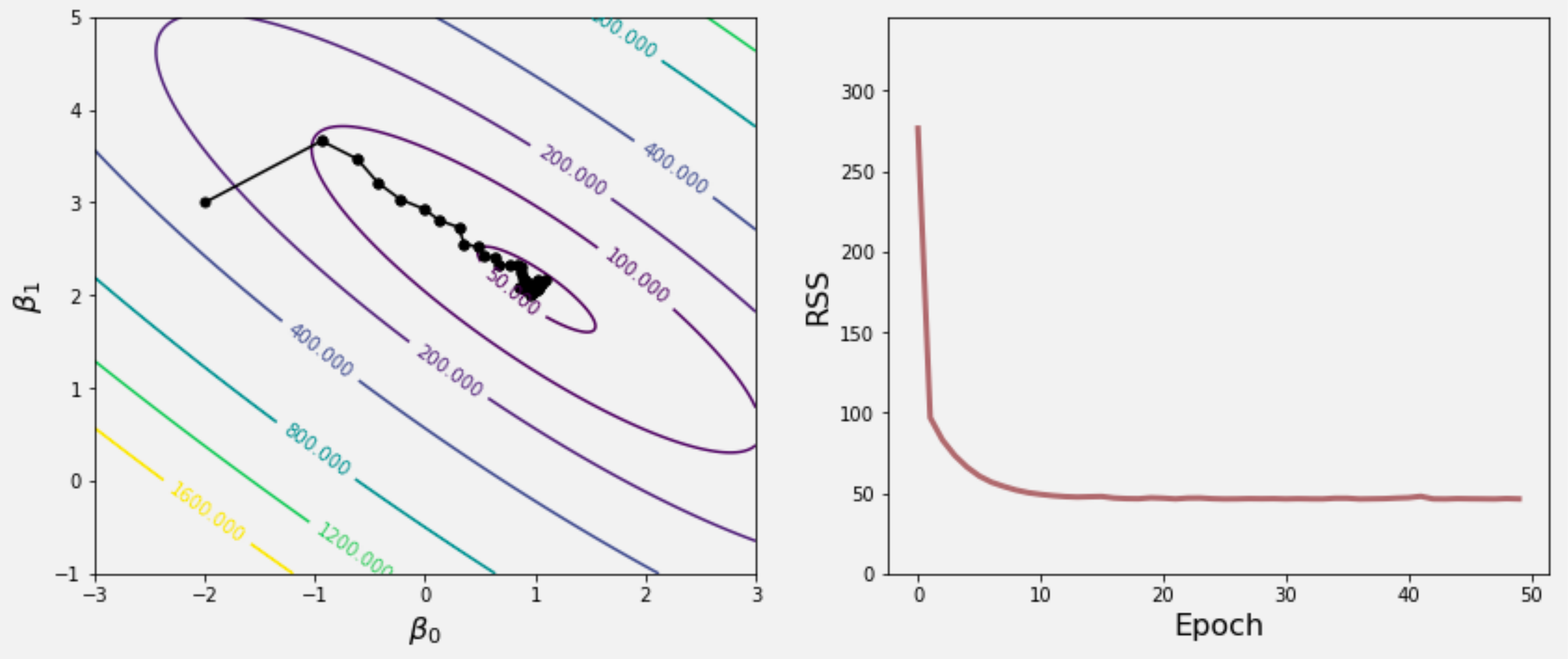
The Importance of the Learning Rate

Way too large a learning rate and you can diverge



The Importance of the Learning Rate

Generally have to tune learning rate to get it just right



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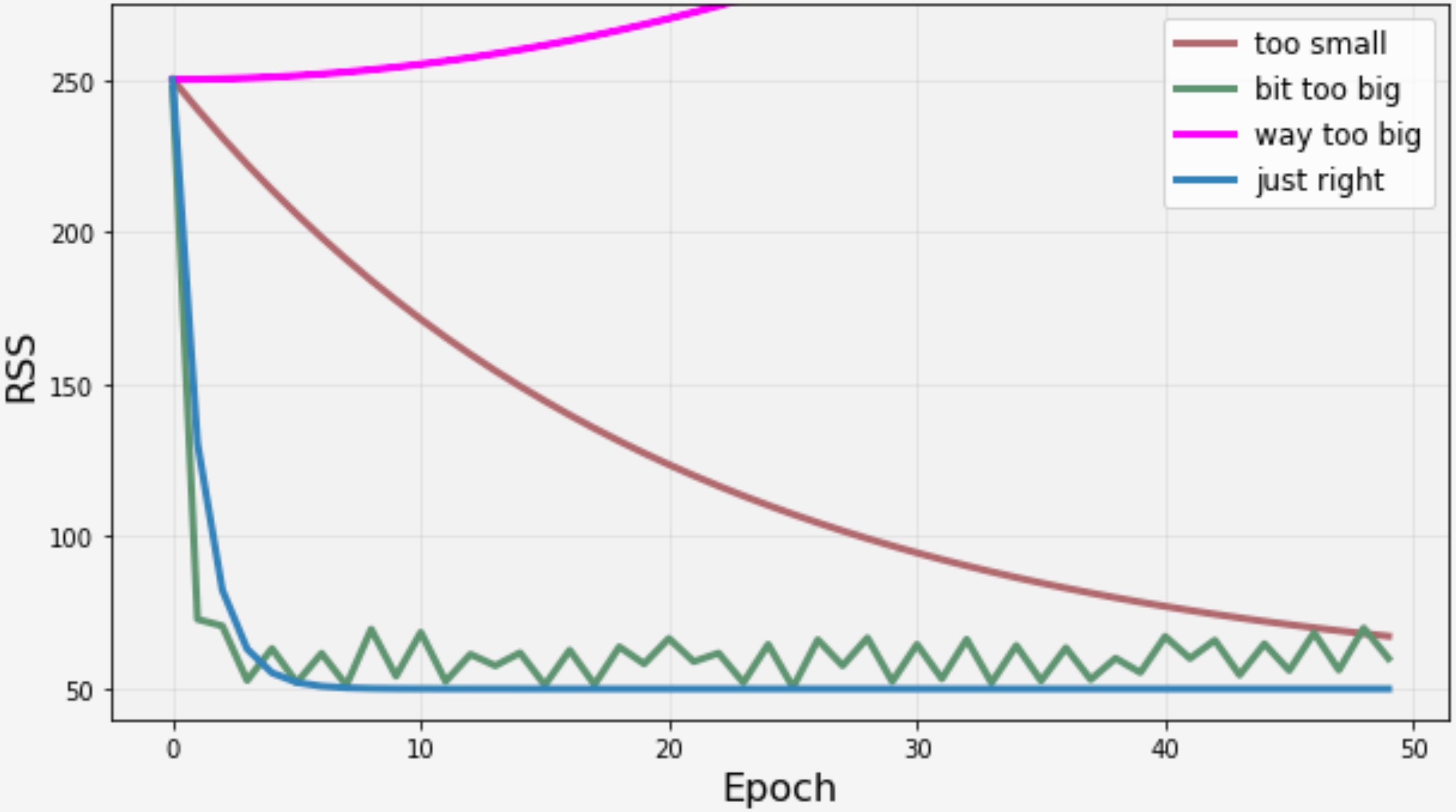

SGD in Higher Dimensions

So far we've looked at SGD for SLR, where we have two parameters

But what about in the more common case of multiple linear regression with p parameters?

$$\text{RSS} = \sum_{i=1}^{n} \left[(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i\right]^2$$

Still has same general form, but now the parameter vector and gradient vector are longer

$$\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \eta \nabla \text{RSS} \quad \Leftrightarrow \quad \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} \leftarrow \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} - \eta \begin{bmatrix} 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i) \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i) x_{i1} \\ \vdots \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i) x_{ip} \end{bmatrix}$$

SGD in Higher Dimensions

What if we want to add regularization? (PSST: We **always** want to add regularization)

$$\mathrm{RSS}_\lambda = \sum_{i=1}^{n} \left[(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i\right]^2 + \lambda \sum_{k=1}^{p} \beta_k^2$$

Only thing that changes is the derivatives of the non-bias parameters

$$\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} \leftarrow \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} - \eta \begin{bmatrix} 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{\mathrm{p}} x_{ip}) - y_i) \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{\mathrm{p}} x_{ip}) - y_i) x_{i1} + 2\lambda\beta_1 \\ \vdots \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{\mathrm{p}} x_{ip}) - y_i) x_{ip} + 2\lambda\beta_p \end{bmatrix}$$

SGD Part I Wrap-Up

- SGD and it's variants are most popular way of training most learning models
- Fairly efficient in time. **Very** efficient in space.
- Lots of little improvements we can do to make more efficient (Hands-On Friday)

Next Time:

- See how we can do SGD for learning the weights in Logistic Regression
- Derive the Logistic Regression loss function via Maximum Likelihood Estimation

If-Time Bonus: Better Vectorization

Recall the Regularized SGD iteration for multiple linear regression

$$\mathrm{RSS}_\lambda = \sum_{i=1}^{n} \left[(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) - y_i \right]^2 + \lambda \sum_{k=1}^{p} \beta_k^2$$

Do you see anything redundant in each term in the gradient?

$$\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} \leftarrow \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} - \eta \begin{bmatrix} 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_1 x_{ip}) - y_i) \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_1 x_{ip}) - y_i) x_{i1} + 2\lambda\beta_1 \\ \vdots \\ 2((\beta_0 + \beta_1 x_{i1} + \cdots + \beta_1 x_{ip}) - y_i) x_{ip} + 2\lambda\beta_p \end{bmatrix}$$