Gradients & Regression

A system of linear equations

Find x_1, x_2, x_3 such that

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

Can also be written as

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

Or as: $\mathbf{Ax} = \mathbf{b}$

To solve, invert the matrix

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

- Inverse might not exist
- System can be
  - under-determined (infinite set of solutions)
  - Or over determined (no solution).

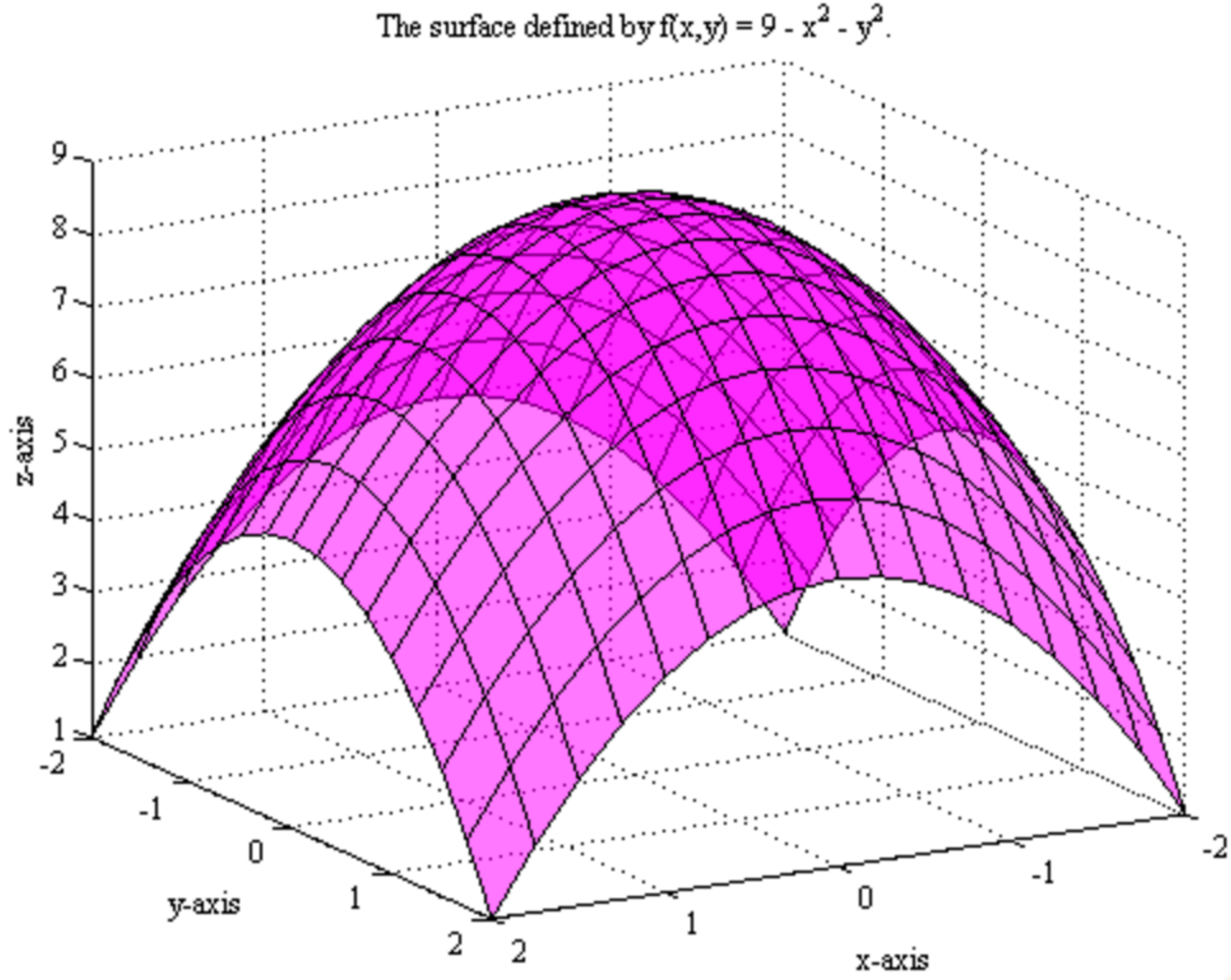
Approximately solving over-determined systems

$$\text{There is no } \mathbf{x} \text{ that satisfies } \mathbf{Ax} = \mathbf{b}$$

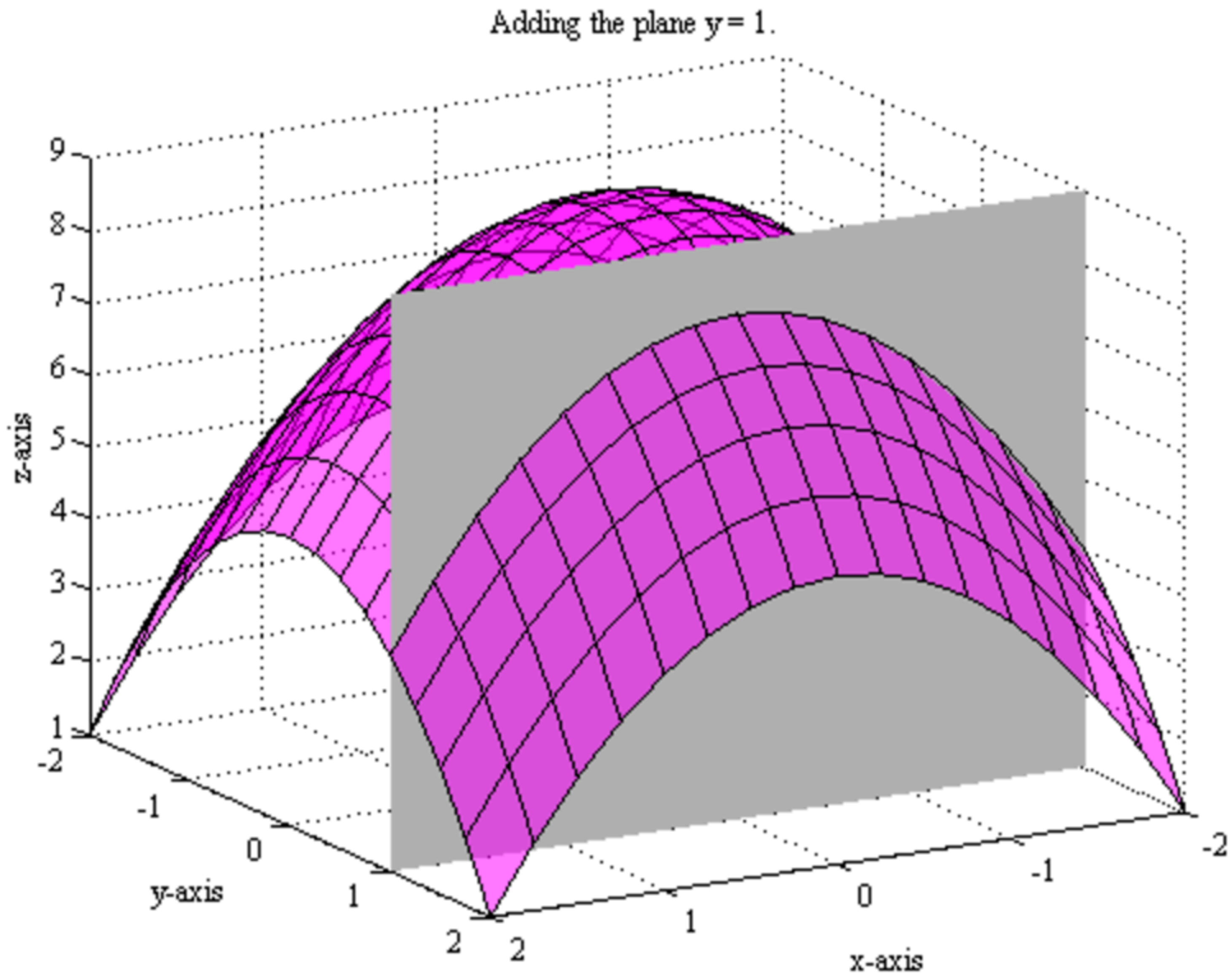
$$\text{Instead, find } \mathbf{x} \text{ that minimizes } \|\mathbf{Ax} - \mathbf{b}\|_2$$

- How to find the minimum?
- In one dimensional problem: set derivative to zero.
- In multi-dimensional case, set **gradient** to zero.

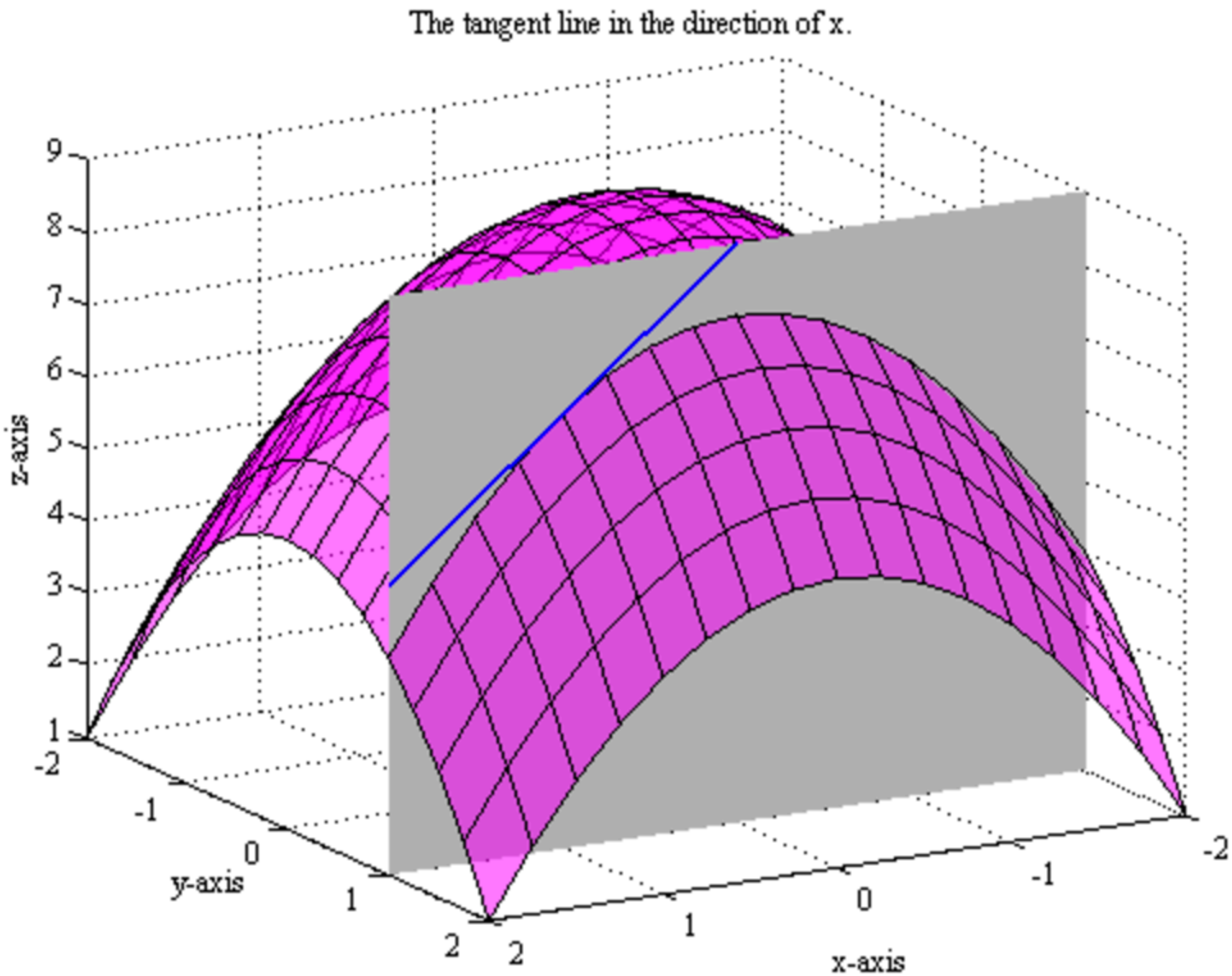
A function of two variables



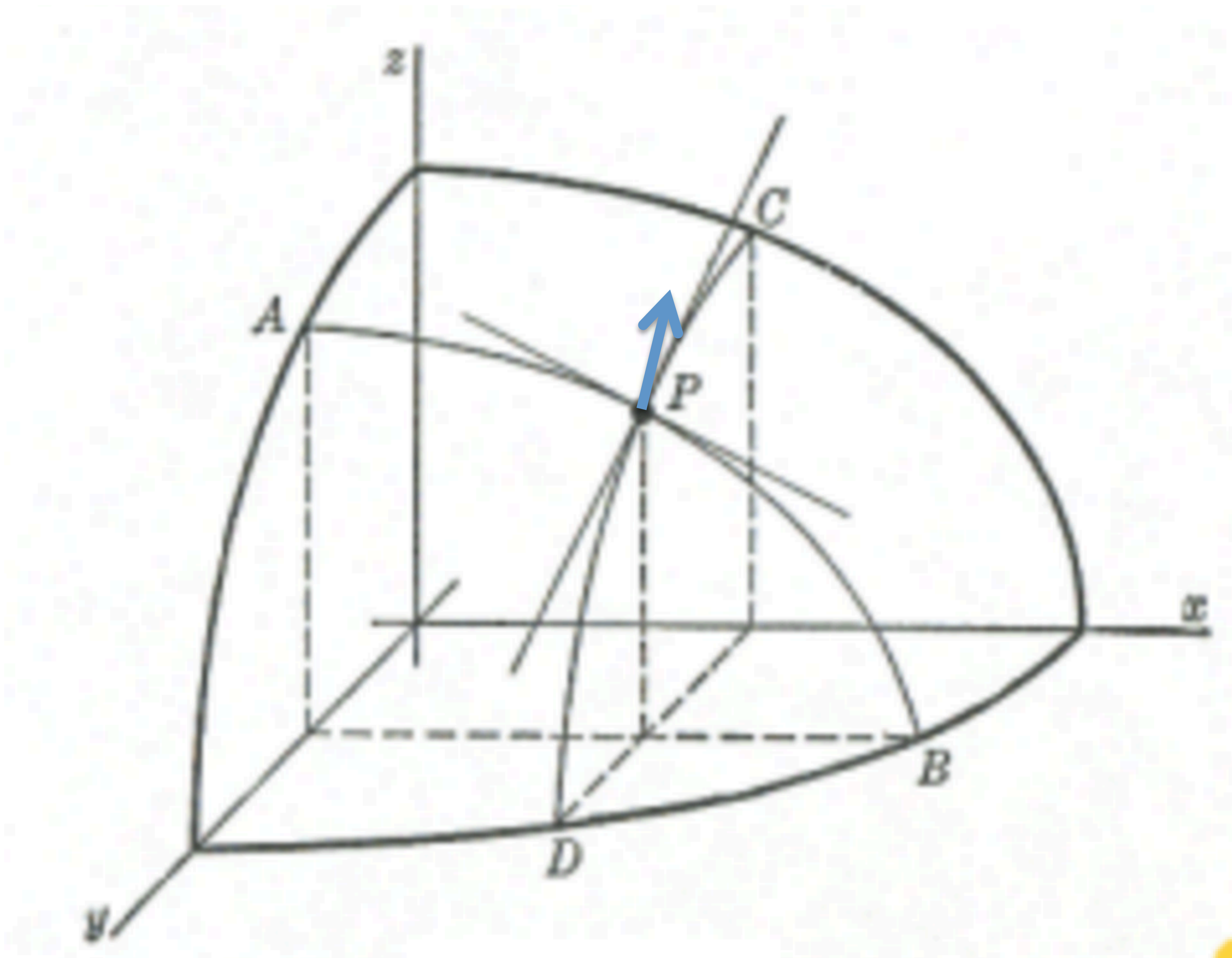
Restricting the function to the variable x



Computing the partial derivative wrt x



Gradient = the partial derivative wrt all coordinates



Computing the gradient symbolically

$$\nabla f = \left\langle \frac{\partial}{\partial x} f, \frac{\partial}{\partial y} f \right\rangle$$

example: $\quad f(x,y) = 9 - x^2 - y^2$

$\nabla f = \langle -2x, -2y \rangle$

Setting the gradient to zero we find that the maximum is at $\langle x,y \rangle = \langle 0,0 \rangle$

Exactly minimizing square error

There is no $\mathbf{x}$ that satisfies $\mathbf{Ax} = \mathbf{b}$

Instead, find $\mathbf{x}$ that minimizes $\|\mathbf{Ax} - \mathbf{b}\|_2^2$

Find $\mathbf{x}$ such that $\nabla_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{b}\|_2^2 = 0$

$$\nabla_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{b}\|_2^2 = 2\mathbf{A}^T(\mathbf{Ax} - \mathbf{b}) = 0$$

$$\mathbf{x} = \underbrace{(\mathbf{A}^{\mathbf{T}}\mathbf{A})^{\mathbf{-1}}\mathbf{A}^{\mathbf{T}}}_{\text{Pseudo-inverse of } \mathbf{A}}\,\mathbf{b}$$

When the number of examples is large

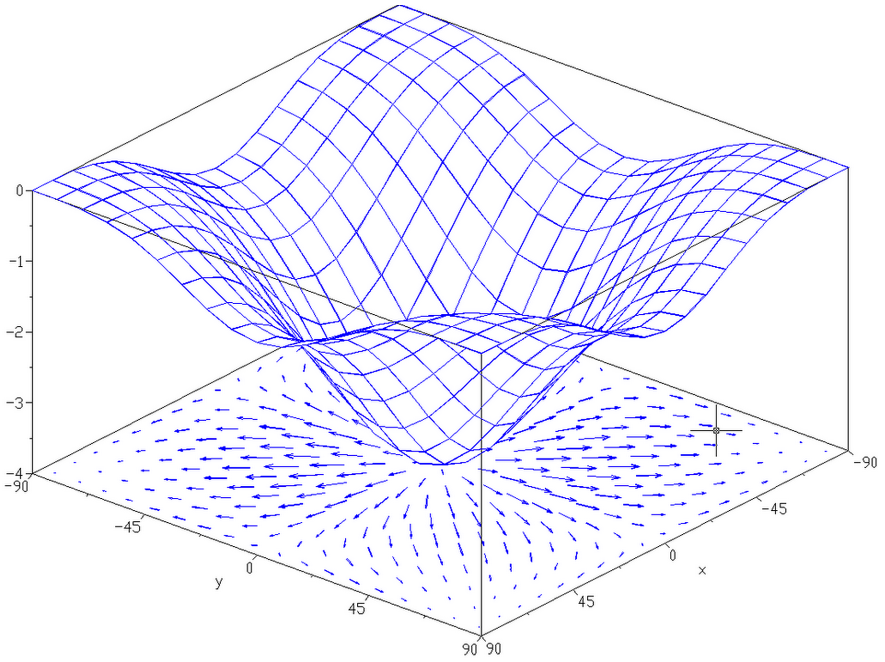
- The size of the matrix **A**
  is number of variables X number of examples
- Exact solution is not practical.
- The alternative: stochastic gradient descent.

Review: the gradient

$f : R^d \to R$ is a smooth function from R^d to R

The gradient of f at the point $\vec{x}$, denoted $\nabla f(\vec{x})$

is a vector pointing in the direction of steepest ascend (increase) of f

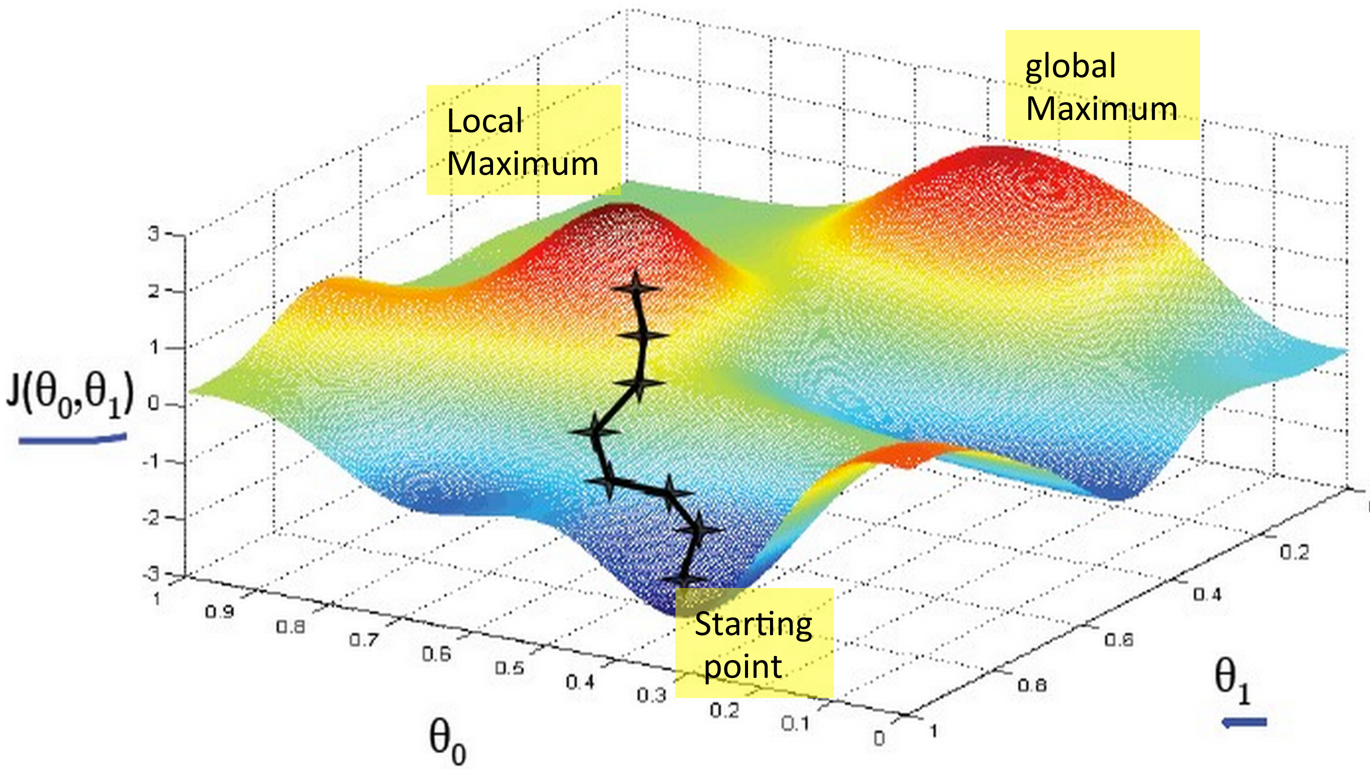


The gradient $\nabla f(\vec{x})$ can be calculated using partial derivatives:

$$\nabla f(\vec{x}) = \left\langle \frac{\partial f(\vec{x})}{\partial x_1}, \frac{\partial f(\vec{x})}{\partial x_2}, \ldots, \frac{\partial f(\vec{x})}{\partial x_d} \right\rangle$$

Optimization by Gradient Ascent

- Start at a randomly chosen starting point
  - Take a small step in the direction of the gradient
  - Repeat
- Converges to a local maximum (gradient zero).
- Which local maximum depends on starting point



Deterministic & Stochastic Gradient Descent

$$\text{Find } \mathbf{x} \text{ that minimizes } \|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^2 = \sum_{i=1}^{N} \left(\mathbf{a}_i\mathbf{x}-b_i\right)^2$$

$$\nabla_{\mathbf{x}} \|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^2 = \nabla_{\mathbf{x}} \sum_{i=1}^{N} \left(\mathbf{a}_i\mathbf{x}-b_i\right)^2 = \sum_{i=1}^{N} 2\left(\mathbf{a}_i\mathbf{x}-b_i\right)\mathbf{a}_i$$

- Taking a step in direction opposite of gradient moves x towards the minimum.
- **Deterministic gradient Descent:** sum over all examples and then take a step.
- **Stochastic Gradient Descent:** take a small step after each example.
- **Mini-Batch:** Take a step after summing M>1 examples.

LinearRegressionWithSGD

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \underbrace{\eta}_{\text{step/ learning rate}} \underbrace{\sum_{i=1}^{M} \underbrace{(\mathbf{a}_{t,i} \cdot \mathbf{x}_t - b_t)}_{\text{error}} \mathbf{a}_{t,i}}_{\text{mini-batch}}$$

LinearRegressionWithSGD(data,it,s,miniB,init)

- **data** – The training data, an RDD of LabeledPoint.
- **iterations** – The number of iterations (default: 100).
- **step** – The step parameter used in SGD (default: 1.0).
- **miniBatchFraction** – Fraction of data to be used for each SGD iteration (default: 1.0).
- **initialWeights** – The initial weights (default: None).

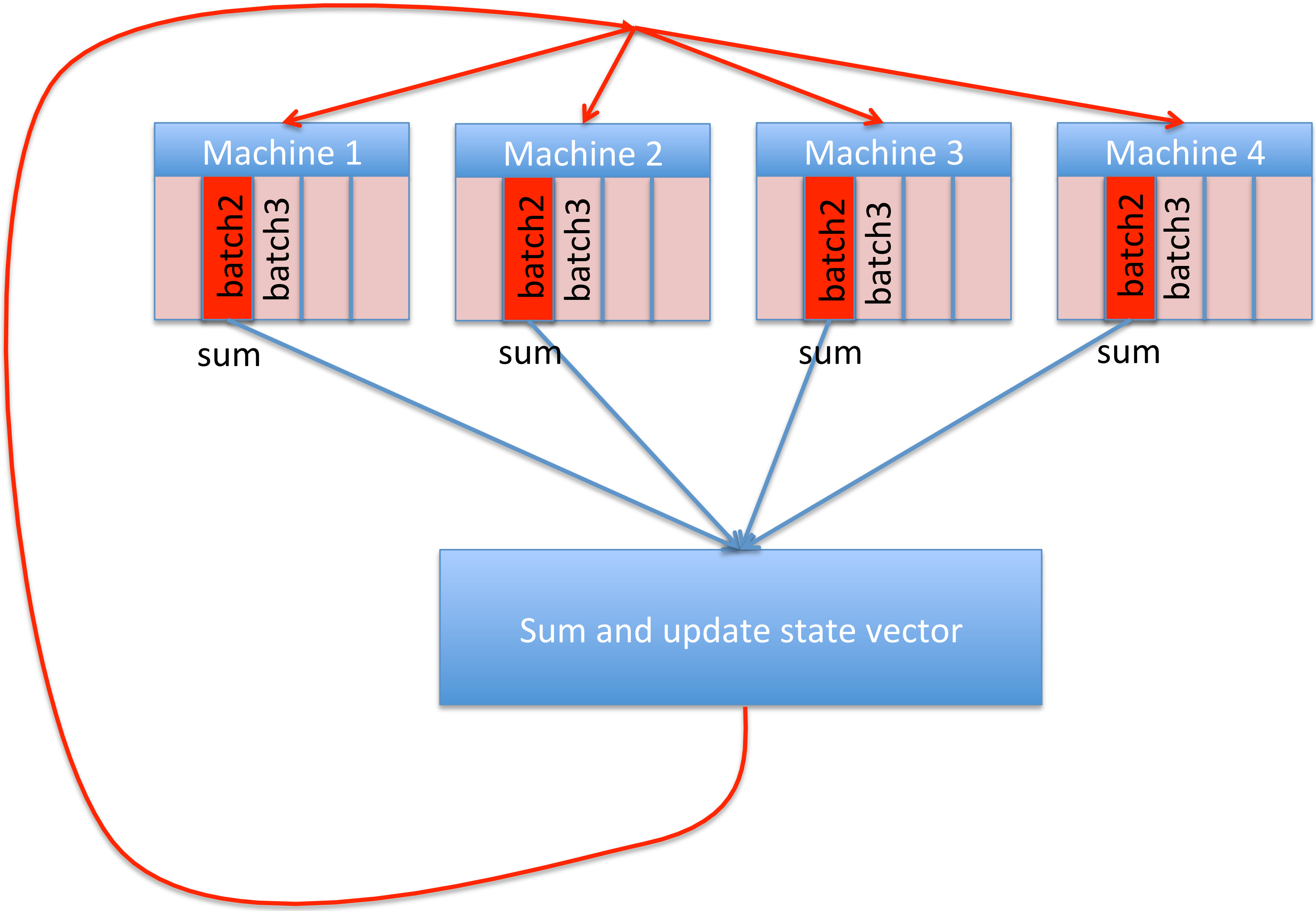
Learning rate and initial weights

- SGD is guaranteed to converge to a local minimum, if the learning rate (step) is sufficiently small.
- If step size too large – SGD can diverge.
- If step size too small – convergence will take many iterations.
- Initial weights can help start the process close to the minimum.

Why Minibatch?

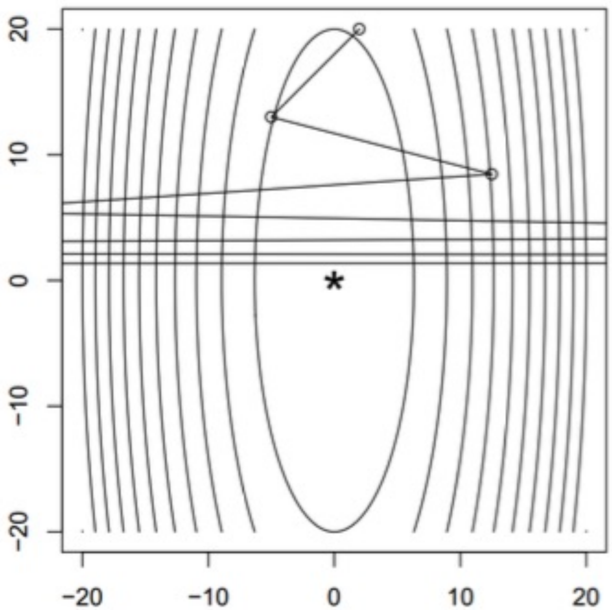
- Updating separately in each executor will cause the estimate of x for different partitions to diverge.
- Alternatively, communicating each update to all executors creates a communication and synchronization bottleneck.
- **Minibatch:** each partition calculates a sum using a fraction of it's partition. The sums are combined and all executors receive the same updated x
- Smaller mini-batches – faster convergence, but more communication.

Mini-Batch SGD

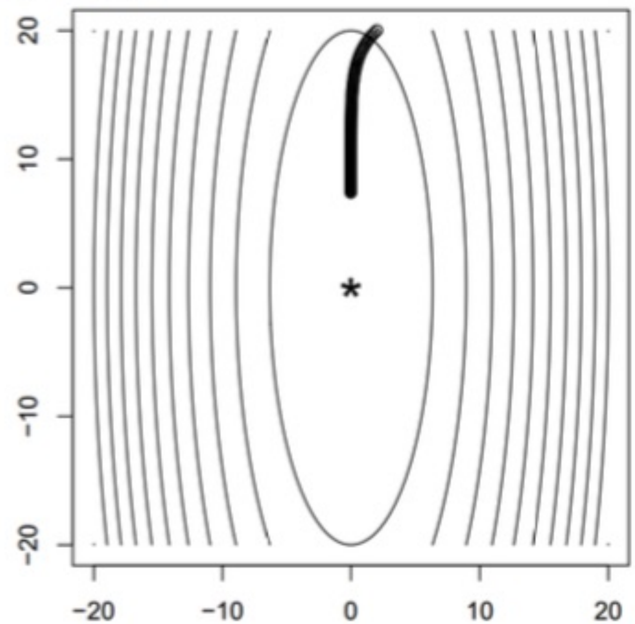


Learning rate matters!

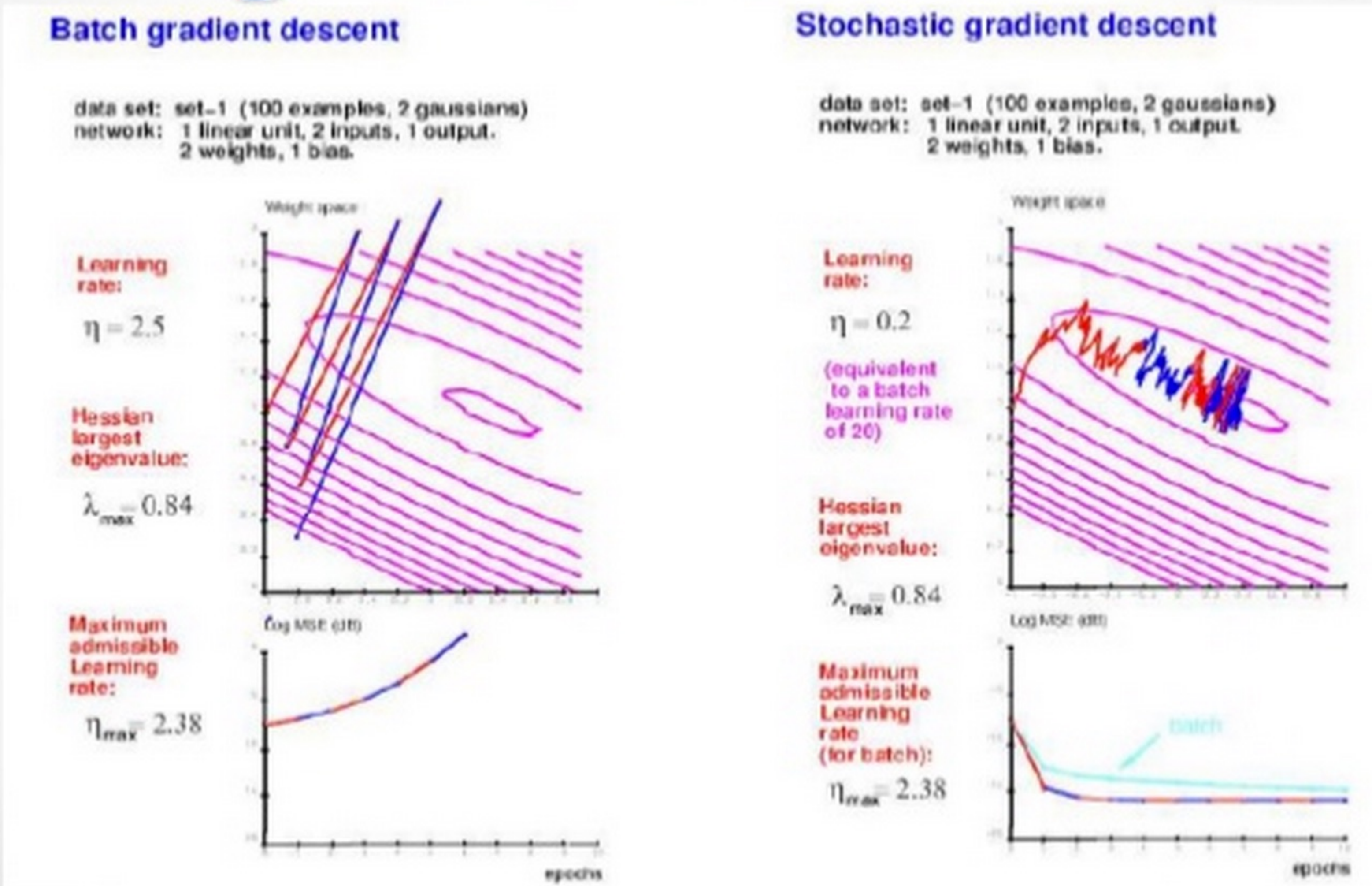
$\eta_t = t$, it is too big



too small η_t, after 100 iterations



Stochastic gradient descent



[LeCun et al, "Efficient BackProp", *Neural Networks: Tricks of the Trade*, 1998;
Bottou, "Stochastic Learning", *Slides from a talk in Tubingen*, 2003]

Training set and Test set

- We are usually interested in finding models that fit well **unseen** data.
- To evaluate the effectiveness of the learning algorithm we separate the data randomly into two parts:
  - Training set: used to find best model
  - Test set: used to see if model generalizes well.

Regularization

- When the data is high dimensional and noisy, decreasing the training error too much will often cause the test error to increase.
- This is called overfitting.
- One way to avoid overfitting is to “regularize” the trained model.

$$\text{Find } \mathbf{x} \text{ that minimizes } \|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^{\,2} + \lambda\|\mathbf{x}\|$$

$$\text{L2: Ridge Regression: } \|\mathbf{x}\|_2^{\,2} = \sum_i x_i^2$$

$$\text{L1: Lasso: } \|\mathbf{x}\|_1 = \sum_i |x_i|$$

Additional Parameters for LinearRegressionWithSGD

- **regParam** – The regularizer parameter (default: 0.0).
- **regType** –
  The type of regularizer used for training our model.
  Allowed values:
  - "l1" for using L1 regularization (lasso),
  - "l2" for using L2 regularization (ridge),
  - None for no regularization

  (default: None)
- **intercept** – Boolean parameter which indicates the use or not of the augmented representation for training data (i.e. whether bias features are activated or not, default: False).
- **validateData** – Boolean parameter which indicates if the algorithm should validate data before training. (default: True)
- **convergenceTol** – A condition which decides iteration termination. (default: 0.001)