Linear Methods for Regression, Optimization

Overview

Linear Regression:

- Task: predict scalar-valued targets (e.g. stock prices)
- Architecture: linear function of the inputs

Modular approach:

1. ***choose a model*** describing the relationships between variables of interest（选择描述我们感兴趣的元素和变量之间关系的模型）
2. ***define a loss function*** quantifying how bad the fit to the data is
3. ***choose a regularizer*** (正则化) saying how much we prefer different candidate models (or explanations of data)
4. fit a model that minimizes the loss function and satisfies the constraint/penalty imposed by the regularizer, possibly using an ***optimization algorithm***

Linear Regression

Model

Model: In linear regression, we use a *linear* function of the features $\mathbf{x} = (x_1, \ldots, x_D) \in \mathbb{R}^D$ to make predictions y of the target value $t \in \mathbb{R}$:

$$y = f(\mathbf{x}) = \sum_j w_j x_j + b$$

- y is the prediction
- $\mathbf{w}$ is the weights
- b is the bias (or intercept)

$\mathbf{w}$ and b together are the parameters

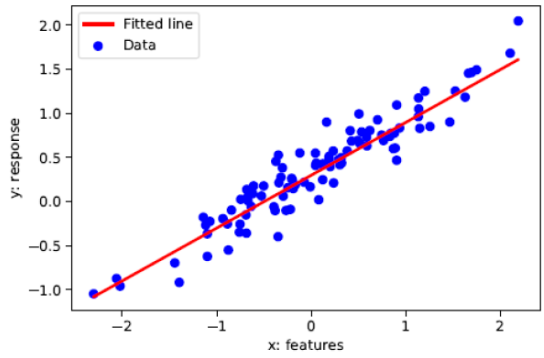
We hope that our prediction is close to the target: $y \approx t$.

Linear Regression

We have a dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)}) \text{ for } i = 1, 2, ..., N\}$ where,

- $\mathbf{x}^{(i)} = (x_1^{(i)}, x_2^{(i)}, ..., x_D^{(i)})^\top \in \mathbb{R}^D$ are the inputs (e.g. age, height)
- $t^{(i)} \in \mathbb{R}$ is the target or response (e.g. income)
- predict $t^{(i)}$ with a linear function of $\mathbf{x}^{(i)}$:

注：$t^{(i)}$ 是对于 $x^{(i)}$ 的预测结果



- $t^{(i)} \approx y^{(i)} = \mathbf{w}^\top \mathbf{x}^{(i)} + b$
- Different $(\mathbf{w}, b)$ define different lines.
- We want the "best" line $(\mathbf{w}, b)$.
- How to quantify "best"?

Loss Function

- A loss function $\mathcal{L}(y, t)$ defines how bad it is if, for some example $\mathbf{x}$, the algorithm predicts y, but the target is actually t.
- Squared error loss function:

$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

注：$y - t$ 是 residual（差距），我们希望它越小越好；

乘以 $\frac{1}{2}$ 可以减轻运算量。

- **Cost function**：所有 training examples 的平均 loss

$$\begin{aligned} \mathcal{J}(\mathbf{w}, b) &= \frac{1}{2N} \sum_{i=1}^{N} \left(y^{(i)} - t^{(i)} \right)^2 \\ &= \frac{1}{2N} \sum_{i=1}^{N} \left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)} \right)^2 \end{aligned}$$

  - 术语不同：有些叫 cost 或 average loss
  - 符号方面：将 $\frac{1}{2N} \sum_{i=1}^{N} \left(y^{(i)} - t^{(i)} \right)^2$ 中的 $y^{(i)}$ 展开会得到

    $$\frac{1}{2N} \sum_{i=1}^{N} \left(\sum_{j=1}^{D} \left(w_j x_j^{(i)} + b \right) - t^{(i)} \right)^2$$

    注：N 指有 N 个 training examples，D 指 x 有 D 个 features

Vectorization

- Computing the predictions for the whole dataset:

$$\mathbf{X}\mathbf{w} + b\mathbf{1} = \begin{pmatrix} \mathbf{w}^T \mathbf{x}^{(1)} + b \\ \vdots \\ \mathbf{w}^T \mathbf{x}^{(N)} + b \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{pmatrix} = \mathbf{y}$$

- Computing the squared error cost across the whole dataset:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}$$
$$\mathcal{J} = \frac{1}{2N}\|\mathbf{y} - \mathbf{t}\|^2$$

- We can also add a column of 1's to design matrix, combine the bias and the weights, and conveniently write

$$\mathbf{X} = \begin{bmatrix} 1 & [\mathbf{x}^{(1)}]^\top \\ 1 & [\mathbf{x}^{(2)}]^\top \\ 1 & \vdots \end{bmatrix} \in \mathbb{R}^{N\times(D+1)} \quad \text{and} \quad \mathbf{w} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix} \in \mathbb{R}^{D+1}$$

Then, our predictions reduce to $\mathbf{y} = \mathbf{X}\mathbf{w}$.

Minimization loss

Two commonly applied mathematical approaches:

- Algebraic (代数方法), e.g. using inequalities (不等式):
  - to show z^* minimizes $f(z)$, show that $\forall z, f(z) \geq f(z^*)$
  - to show that $a = b$, show that $a \geq b$ and $b \geq a$
- Calculus: minimum of a smooth function (if it is exists) occurs at a critical point (临界点), i.e. point where the derivative is zero (导数为零的点).

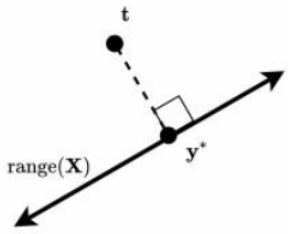
Solutions may be direct or iterative.

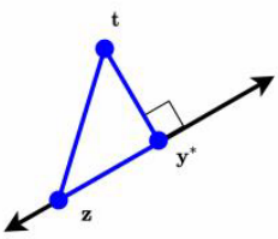
Direct Solution

Linear Algebra

我们要寻找一个 w 来 minimize $\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$, or equivalently $\|\mathbf{X}\mathbf{w} - \mathbf{t}\|$.
$\text{range}(\mathbf{X}) = \{\mathbf{X}\mathbf{w} \mid \mathbf{w} \in \mathbb{R}^D\}$ is a D-dimensional subspace of $\mathbb{R}^N$.

The closest point $\mathbf{y}^* = \mathbf{X}\mathbf{w}^*$ in subspace range$(\mathbf{X})$ of $\mathbb{R}^N$ to arbitrary point $\mathbf{t} \in \mathbb{R}^N$ is found by orthogonal projection (直角投影).





- We have $(\mathbf{y}^* - \mathbf{t}) \perp \mathbf{X}\mathbf{w},\ \forall \mathbf{w} \in \mathbb{R}^D$
- Why is $\mathbf{y}^*$ the closest point to $\mathbf{t}$?
  - Consider any $\mathbf{z} = \mathbf{X}\mathbf{w}$
  - By Pythagorean theorem and the trivial inequality $(x^2 \geq 0)$:

$$\begin{aligned}\|\mathbf{z} - \mathbf{t}\|^2 &= \|\mathbf{y}^* - \mathbf{t}\|^2 + \|\mathbf{y}^* - \mathbf{z}\|^2 \\ &\geq \|\mathbf{y}^* - \mathbf{t}\|^2\end{aligned}$$

注：range(**X**) 和它所在的线，代表的是可能的 y 值。

- From the previous slide, we have $(\mathbf{y}^* - \mathbf{t}) \perp \mathbf{X}\mathbf{w},\ \forall \mathbf{w} \in \mathbb{R}^D$
- Equivalently, the columns of the design matrix $\mathbf{X}$ are all orthogonal to $(\mathbf{y}^* - \mathbf{t})$, and we have that:

$$\begin{aligned} \mathbf{X}^\top(\mathbf{y}^* - \mathbf{t}) &= \mathbf{0} \\ \mathbf{X}^\top\mathbf{X}\mathbf{w}^* - \mathbf{X}^\top\mathbf{t} &= \mathbf{0} \\ \mathbf{X}^\top\mathbf{X}\mathbf{w}^* &= \mathbf{X}^\top\mathbf{t} \\ \mathbf{w}^* &= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{t} \end{aligned}$$

Calculus

- Partial derivative: derivative of a multivariate function with respect to one of its arguments.

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

- For cost derivatives, use linearity and average over data points:

$$\frac{\partial \mathcal{J}}{\partial w_j} = \frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, x_j^{(i)} \qquad \frac{\partial \mathcal{J}}{\partial b} = \frac{1}{N} \sum_{i=1}^{N} y^{(i)} - t^{(i)}$$

注：这里是对 w，和 b 的偏导。

- Minimum must occur at a point where partial derivatives are zero.

$$\frac{\partial \mathcal{J}}{\partial w_j} = 0 \quad (\forall j), \qquad \frac{\partial \mathcal{J}}{\partial b} = 0.$$

(if $\partial \mathcal{J} / \partial w_j \neq 0$, you could reduce the cost by changing w_j)

- We call the vector of partial derivatives the gradient
- Thus, the "gradient of $f : \mathbb{R}^D \to \mathbb{R}$", denoted $\nabla f(\mathbf{w})$, is:

$$\left(\frac{\partial}{\partial w_1} f(\mathbf{w}), \ldots, \frac{\partial}{\partial w_D} f(\mathbf{w}) \right)^\top$$

注：上式是 w 的梯度。

梯度的方向，和函数最大增长率的方向一致。

Analogue (类似情况) of second derivative (the "Hessian" matrix): $\nabla^2 f(\mathbf{w}) \in \mathbb{R}^{D \times D}$ is a matrix with $\left[\nabla^2 f(\mathbf{w})\right]_{ij} = \frac{\partial^2}{\partial w_i \partial w_j} f(\mathbf{w})$

注：海森矩阵，描述了函数的局部曲率，可判定多元函数的极值问题。用二次导数，可以确定梯度的变化趋势。

- We seek $\mathbf{w}$ to minimize $\mathcal{J}(\mathbf{w}) = \frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$
- Taking the gradient with respect to $\mathbf{w}$ (**see course notes for additional details**) we get:

$$\nabla_{\mathbf{w}}\mathcal{J}(\mathbf{w}) = \mathbf{X}^\top\mathbf{X}\mathbf{w} - \mathbf{X}^\top\mathbf{t} = \mathbf{0}$$

- We get the same optimal weights as before:

$$\mathbf{w}^* = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{t}$$

注：矩阵求导不能用链式法则，有特殊的规则，因此：

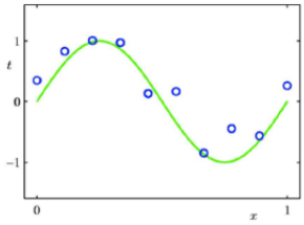
$$\begin{aligned}\nabla_w\mathcal{J}(w) &= \frac{1}{2}\left(X^2w^2 + t^2 - 2Xwt\right)' \\ &= \frac{1}{2}\left(2X^2w - 2Xt\right) \\ &= X^2w - Xt \\ &= X^\top Xw - X^\top t\end{aligned}$$

Feature Mapping (Basis Expansion)

不是所有输入和输出的关系都是线性的，更多的可能是多项式关系 (polynomial relation)。如果样本量多，回归问题很复杂，而原始特征只有x1,x2。可以用多项式创建更多的特征x1、x2、$x1^2$、$x2^2$、... 。因为更多的特征进行回归时，得到的分割线可以是任意高阶函数的形状。

通过一定的映射，把数据映射入高维之后，便于分界。因为保留了映射前的特征，所以叫特征映射。

If the relationship doesn't look linear, we can fit a polynomial.



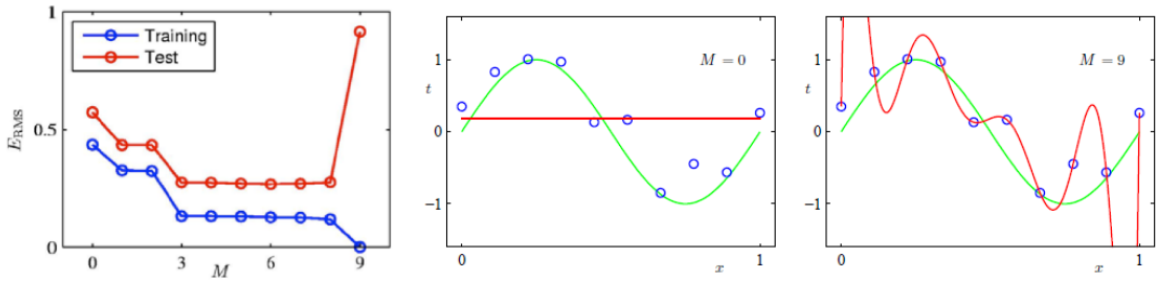
Fit the data using a degree-M polynomial function of the form:

$$y = w_0 + w_1x + w_2x^2 + ... + w_Mx^M = \sum_{i=0}^{M} w_ix^i$$

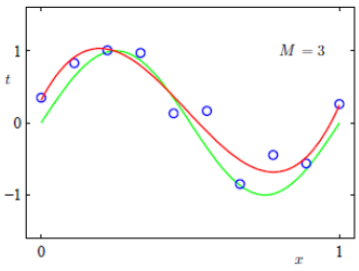
- Here the feature mapping is $\boldsymbol{\psi}(x) = [1, x, x^2, ..., x^M]^\top$.
- We can still use linear regression to find $\mathbf{w}$ since $y = \boldsymbol{\psi}(x)^\top\mathbf{w}$ is linear in $w_0, w_1, ...$
- In general, $\boldsymbol{\psi}$ can be any function. Another example: $\boldsymbol{\psi}(x) = [1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), ...]^\top$.

注：在这个问题中，input 只有一个 feature，就是 x 轴的值。将这个feature 映射到 M 个维度中，就得到了上式。

Underfitting (M=0): model is too simple — does not fit the data.
Overfitting (M=9): model is too complex — fits perfectly.



Good model (M=3): Achieves small test error (generalizes well).



Regularization

多项式的 degree M 控制了模型的复杂度。M 是一个超参数，和 KNN 中的 k 一样，因此我们同样可以使用 validation set 来进行调整。

不过，我们还有另外的方法：keep the model large, but ***regularize*** it

- **Regularizer**: a function that quantifies how much we prefer one hypothesis vs. another

L2 Regularization

我们可以选择使用 **L^2 penalty** 作为 regularizer 来使 weights 变小。

$$\mathcal{R}(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2 = \frac{1}{2}\sum_j w_j^2$$

正则化的代价函数（regularized cost function）在 数据的拟合 和 权重的范数（norm of the weights） 之间进行权衡。

$$\mathcal{J}_{\mathrm{reg}}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \lambda\mathcal{R}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \frac{\lambda}{2}\sum_j w_j^2$$

- If you fit training data poorly, $\mathcal{J}$ is large (误差大). If your optimal weights have high values, $\mathcal{R}$ is large (模型复杂).
- Large λ penalizes weight values more.
- 和 M 一样， λ 也是 hyperparameter，可以通过 validation set 调整

L2 Regularized Least Squares: Ridge regression

For the least squares problem, we have $\mathcal{J}(\mathbf{w}) = \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$.

- When $\lambda > 0$ (with regularization), regularized cost gives

$$\mathbf{w}_\lambda^{\text{Ridge}} = \underset{\mathbf{w}}{\text{argmin}}\, \mathcal{J}_{\text{reg}}(\mathbf{w}) = \underset{\mathbf{w}}{\text{argmin}}\, \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$
$$= (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}$$

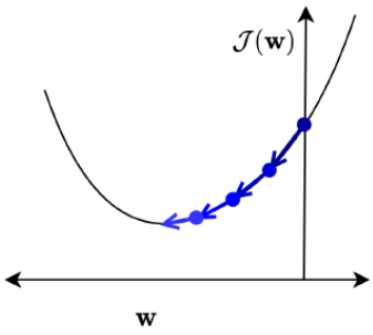
- The case $\lambda = 0$ (no regularization) reduces to least squares solution!
- Note that it is also common to formulate this problem as $\text{argmin}_{\mathbf{w}}\, \frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$ in which case the solution is $\mathbf{w}_\lambda^{\text{Ridge}} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}$.

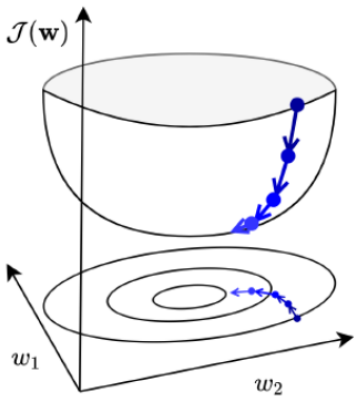
注：$\mathbf{I}$ 表示单位矩阵，即在主对角线上元素均为 1，而其他元素都是 0

Gradient Descent

很多时候，我们没有 direct solution。

Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.





- Observe:
  - if $\partial \mathcal{J}/\partial w_j > 0$, then increasing w_j increases $\mathcal{J}$.
  - if $\partial \mathcal{J}/\partial w_j < 0$, then increasing w_j decreases $\mathcal{J}$.
- The following update always decreases the cost function for small enough α (unless $\partial \mathcal{J}/\partial w_j = 0$):

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j}$$

- $\alpha > 0$ is a learning rate (or step size). The larger it is, the faster $\mathbf{w}$ changes.
  - We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001.
  - If cost is the sum of N individual losses rather than their average, smaller learning rate will be needed ($\alpha' = \alpha/N$).
- This gets its name from the gradient:

$$\nabla_{\mathbf{w}} \mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

  - This is the direction of fastest increase in $\mathcal{J}$.
- Update rule in vector form:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

  And for linear regression we have:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, \mathbf{x}^{(i)}$$

- So gradient descent updates $\mathbf{w}$ in the direction of fastest *decrease*.
- Observe that once it converges, we get a critical point, i.e. $\frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \mathbf{0}$.

Gradient Descent under the L2 Regularization

- Gradient descent update to minimize $\mathcal{J}$:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} \mathcal{J}$$

- The gradient descent update to minimize the L^2 regularized cost $\mathcal{J} + \lambda \mathcal{R}$ results in weight decay:

$$\begin{aligned}
\mathbf{w} &\leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} (\mathcal{J} + \lambda \mathcal{R}) \\
&= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right) \\
&= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right) \\
&= (1 - \alpha\lambda)\mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}
\end{aligned}$$

Stochastic Gradient Descent

- So far, the cost function $\mathcal{J}$ has been the average loss over the training examples:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}^{(i)} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(y(\mathbf{x}^{(i)}, \boldsymbol{\theta}), t^{(i)}).$$

  ($\boldsymbol{\theta}$ denotes the parameters; e.g., in linear regression, $\boldsymbol{\theta} = (\mathbf{w}, b)$)

- By linearity,

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}.$$

计算梯度需要计算所有的 training example，这称为 **batch training**。

batch training 有时是不切实际的，如果你有一个大的数据集 $N \gg 1$（例如数百万个 training examples）。

随机梯度下降 （SGD）： 根据单个 training example 的梯度更新参数：

- 均匀随机地选择 i（i 是数据集中的一个 example）
- $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}$

每个 SGD 更新的成本都与 N 无关，SGD 甚至在看到所有数据之前就可以取得重大进展。

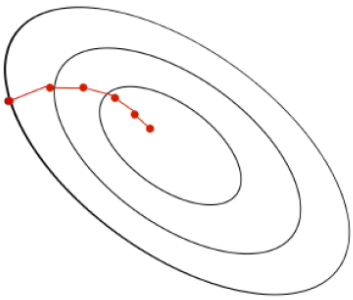
数学理由：如果随机均匀地采样出一个 training example，随机梯度是对批次梯度（batch gradient）的公正估计（unbiased estimate）：

$$\mathbb{E}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} \right] = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}$$

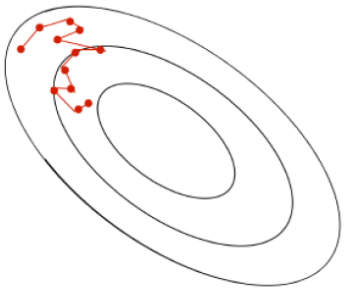
注：上式是对 batch gradient 的估计，结果和前面 By linearity 一致，所以是 unbiased estimate。

使用单一的 training example 来估计梯度可能方差会很高，我们可以随机选择中等大小的数据集 $\mathcal{M} \subset \{1, \ldots, N\}$（称为 mini-batch），来进行训练，而这会使方差变小。

Batch gradient descent moves directly downhill (locally speaking). SGD takes steps in a noisy direction, but moves downhill on average.



batch gradient descent



stochastic gradient descent

SGD Learning Rate

在随机训练（stochastic training）中，学习率也会由于梯度的随机性而影响波动（fluctuations）。

训练策略：

- 在训练的早期使用高学习率，以便快速接最优解
- 逐渐降低学习率，减少 fluctuations