

HOW MANY MC SIMULATIONS?

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CONTENTS

1	Introduction	3
2	Non-Overdispersed	3
2.1	Estimator	3
2.2	Confidence Interval	3
2.3	Example	4
3	Overdispersed	4
3.1	Estimator	4
3.2	Confidence Interval	7
3.3	Example	9
4	Results and Discussion	10
4.1	Subsection	10
4.2	Figure Composed of Subfigures	12

LIST OF FIGURES

Figure 1	An example of a floating figure	11
Figure 2	A number of pictures.	13

LIST OF TABLES

Table 1	Table of N satisfying (3) for different n	10
Table 2	Table of N satisfying 95% confidence interval for different γ, α, β, n	10
Table 3	Table of Grades	12

ABSTRACT

When evaluating Baseball matches using Monte Carlo simulations, we would like to know exactly how many simulations it is necessary to perform. For example lets say we wanted to know the probability of the home team beating the away team to 3 decimal places with probability 95%. Certainly, if we know the distribution of the estimator for our probability (where the variance will depend on the total number of simulations N), then its possible to find the value of N necessary for our estimate

to be within the given confidence interval. This article is concerned with deriving these distributions along with calculating some realistic examples.

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1 INTRODUCTION

When looking to evaluate an event (e.g. home team beats away team by 0.5), each Monte Carlo simulation is essentially a realisation from a Bernoulli random variable, with values of 1 if the event occurred or 0 otherwise. The probability of course is unknown. We consider two cases, first where the probability is assumed to be a fixed point, which we call the non-overdispersed case. This arises when all our Monte Carlo simulations come from the same model. We also consider the overdispersed case, where the probability is assumed to follow a Beta distribution. This arises in our case where we have underlying uncertainty about the skills of the players in our Baseball games. Hence different samples of the players' uncertainties give rise to different models that we Monte Carlo simulate from. Each of these models would have a different associated probability (which we have assumed to be Beta distributed).

In the non-overdispersed case, the only parameter we care about is the total number of simulations for the model n and the value that we should choose to get our event probability estimate within some confidence region. However in the overdispersed case we have two parameters. Again n represents the number of simulations for an individual model but importantly we also have parameter N which represents how many different models we sample, so in total we perform $N \cdot n$ simulations.

As we have an overhead for creating a model, the time taken in the non-overdispersed case is $n + \delta$ and for the overdispersed case $N \cdot (n + \delta)$ where δ represents our overhead. Note then in the non-overdispersed case we can directly solve for n when given a confidence interval we wish to be within with some probability. However in the overdispersed case we will instead have two confidence intervals, one for the mean of the probability and another for the variance of the probability. The problem to solve we then be an optimisation, to find the values of N, n that minimise time $N \cdot (n + \delta)$ such that both the mean and variance estimates are within the given confidence intervals.

2 NON-OVERDISPERSED

In this case we assume the following model. Let our event be represented by random variable X such that

$$X \sim \text{Bernoulli}(p)$$

where p is a fixed point.

2.1 Estimator

Consider n iid random variables with the same distribution as X (representing our Monte Carlo simulations) X_1, \dots, X_n . Then we use the following estimator

$$\hat{P} = \frac{1}{n} \sum_{i=1}^n X_i$$

which by the central limit theorem (CLT) has the following distribution as $n \rightarrow \infty$,

$$\hat{P} \sim \mathcal{N}\left(\mathbb{E}[X], \frac{\text{var}(X)}{n}\right) = \mathcal{N}\left(p, \frac{p(1-p)}{n}\right)$$

2.2 Confidence Interval

Assume we now want to know \hat{P} within some region with a certain probability i.e.

$$\Pr(\hat{P} \in (p - \gamma, p + \gamma) | n) = 1 - \epsilon.$$

Given $\epsilon \in [0, 1]$ and $\gamma > 0$, we wish to solve the above equation for n . Well assuming as in the limit that \hat{P} follows a normal distribution, then we have

$$\Phi\left(\frac{\gamma\sqrt{n}}{\sqrt{p(1-p)}}\right) - \Phi\left(\frac{-\gamma\sqrt{n}}{\sqrt{p(1-p)}}\right) = 1 - \epsilon$$

where Φ is the cdf of a standard normal distribution. Using the symmetry of the normal distribution about 0,

$$\Phi\left(\frac{\gamma\sqrt{n}}{\sqrt{p(1-p)}}\right) = 1 - \epsilon/2$$

2.3 Example

Let's use the case mentioned in the abstract, where we want to know the event to 3 decimal place with probability 95%. In this case we have

$$\epsilon = 0.05$$

and

$$\gamma = 0.0005.$$

We must also set a value for the true probability which we take as

$$p = 0.5.$$

Plugging into our equation we get

$$\Phi\left(\frac{0.0005\sqrt{n}}{0.5}\right) = 0.975$$

$$\Rightarrow n \approx 3841600$$

where we used $\Phi^{-1}(0.975) = 1.96$.

This says we need roughly 4,000,000 simulations to get the desired level of accuracy.

3 OVERDISPERSED

The overdispersed version is a lot more complex than the non-overdispersed version. The model again assumes that our event is represented by random variable X such that

$$X \sim \text{Bernoulli}(P)$$

but in this case P is also a random variable

$$P \sim \text{Beta}(\alpha, \beta).$$

The reason we do this is because as mentioned before, our player skills form a large multivariate normal distribution. Hence to perform our Monte Carlo simulations we must first sample the skills (which we can think of as like sampling a p from P). Then we can perform our Bernoulli simulations, sampling x from $X|P = p$.

3.1 Estimator

First we begin by defining the random variables that we use. Consider

$$P_i \sim \text{Beta}(\alpha, \beta)$$

for $i = 1 \dots N$,

$$X_{ij} \sim \text{Bernoulli}(P_i)$$

for $j = 1 \dots n$ and

$$Z_i = \sum_{j=1}^n X_{ij} \sim \text{Binomial}(n, P_i).$$

Given the X_{ij} and therefore the Z_i , we wish to build estimators for

$$\mathbb{E}[P_i] = \mathbb{E}[P] = \frac{\alpha}{\alpha + \beta}$$

and

$$\text{var}(P_i) = \text{var}(P) = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}$$

which are simply results from Beta distributions.

3.1.1 Moments

To build the estimators we calculate asymptotic distributions for the estimated raw moments of the Z_i/n (where Z_i follow a Beta-Binomial distribution) and combine these together.

The first raw moment estimator is given by

$$\hat{\mu}_1 = \frac{1}{N} \sum_{i=1}^N \frac{Z_i}{n} \sim \mathcal{N}\left(\frac{\mathbb{E}[Z_i]}{n}, \frac{\text{var}(Z_i)}{Nn^2}\right)$$

as $N \rightarrow \infty$ by the CLT. Using the fact that Z_i is Beta-Binomial distributed we know the moment generating function is the generalised hypergeometric function

$$M(t) = {}_2F_1(-n, \alpha; \alpha + \beta; 1 - \exp(t))$$

and therefore

$$m_k(\alpha, \beta, n) = \mathbb{E}[Z_i^k] = M^{(k)}(t)|_{t=0}.$$

This means that they may not be pretty, but we can calculate a fixed form for all the moments of the Beta-Binomial. Hence as $N \rightarrow \infty$,

$$\hat{\mu}_1 \sim \mathcal{N}\left(\frac{\alpha}{\alpha + \beta}, \frac{m_2(\alpha, \beta, n) - m_1(\alpha, \beta, n)^2}{Nn^2}\right).$$

The second raw moment estimator is given by

$$\hat{\mu}_2 = \frac{1}{N} \sum_{i=1}^N \frac{Z_i^2}{n^2} \sim \mathcal{N}\left(\frac{\mathbb{E}[Z_i^2]}{n^2}, \frac{\text{var}(Z_i^2)}{Nn^4}\right)$$

as $N \rightarrow \infty$. In our Beta-Binomial moment notation, this can be written

$$\hat{\mu}_2 \sim \mathcal{N}\left(\frac{m_2(\alpha, \beta, n)}{n^2}, \frac{m_4(\alpha, \beta, n) - m_2(\alpha, \beta, n)^2}{Nn^4}\right).$$

3.1.2 Combining

Now let's see how to combine $\hat{\mu}_1$ and $\hat{\mu}_2$ to get unbiased estimators for $\mathbb{E}[P]$ and $\text{var}(P)$ with known asymptotic distributions. The first case is easy as clearly

$$\mathbb{E}[\hat{\mu}_1] = \mathbb{E}[P]$$

and we know the asymptotic distribution of $\hat{\mu}_1$. Hence we can use the combining function

$$u(\hat{\mu}_1, \hat{\mu}_2) = \hat{\mu}_1$$

as our estimator of $\mathbb{E}[P]$.

The second case is not so easy but we claim the following is an *asymptotically* unbiased estimator of $\text{var}(P)$,

$$v(\hat{\mu}_1, \hat{\mu}_2) = \frac{n\hat{\mu}_2 - \hat{\mu}_1 - (n-1)\hat{\mu}_1^2}{n-1}$$

We write the important lines of the expansion but not that most of the algebra simplification was done by the Sympy package in Python.

$$\begin{aligned} \mathbb{E}[v(\hat{\mu}_1, \hat{\mu}_2)] &= \frac{\frac{m_2}{n} - \frac{m_1}{n} - (n-1)[\text{var}(\hat{\mu}_1) + \mathbb{E}[\hat{\mu}_1]^2]}{n-1} \\ &= \frac{\frac{m_2}{n} - \frac{m_1}{n} - (n-1)(\frac{m_1}{n})^2}{n-1} - \frac{m_2 - m_1}{Nn^2} \\ &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} - \frac{m_2 - m_1}{Nn^2} \\ &= \text{var}(P) - \frac{m_2 - m_1}{Nn^2} \end{aligned}$$

If we expand the second term (without the N term) we find

$$\frac{m_2 - m_1}{n^2} = \frac{n-1}{n} \frac{\alpha(\alpha+1)}{(\alpha + \beta)(\alpha + \beta + 1)} \in (0, 1)$$

where as $\alpha, \beta > 0$ we see the smallest value the term can take is 0 when $\alpha \rightarrow 0$ and the largest is 1 when $\beta \rightarrow 0$ and $n \rightarrow \infty$.

Hence we have that

$$\text{var}(P) \in (\mathbb{E}[v], \mathbb{E}[v] + \frac{1}{N})$$

where we dropped the $\hat{\mu}_1, \hat{\mu}_2$ terms for clearer notation. Hence as $N \rightarrow \infty$, v is an unbiased estimator for $\text{var}(P)$.

Note that it may be preferable to define our estimator as

$$\hat{v} = v + \frac{1}{2N}$$

so that

$$\text{var}(P) \in (\mathbb{E}[\hat{v}] - \frac{1}{2N}, \mathbb{E}[\hat{v}] + \frac{1}{2N})$$

or equivalantly

$$\mathbb{E}[\hat{v}] \in (\text{var}(P) - \frac{1}{2N}, \text{var}(P) + \frac{1}{2N})$$

a symmetric interval. Of course this is then also asymptotically unbiased and has the same variance as v . The real benefit comes however with confidence intervals as now let's say we want to know our estimator \hat{v} is within $\text{var}(p)$ with *at least* 95% probability say. Then we want to find γ such that

$$\Pr(\hat{v} \in (\text{var}(P) - \gamma, \text{var}(P) + \gamma)) > 95\%.$$

Well we can find (using our asymptotic distribution) γ such that,

$$\Pr(\hat{v} \in (\mathbb{E}[\hat{v}] - \gamma + \frac{1}{2N}, \mathbb{E}[\hat{v}] + \gamma - \frac{1}{2N})) = 95\%$$

and therefore using the fact

$$\hat{v} > \mathbb{E}[\hat{v}] - \gamma + \frac{1}{2N} > \text{var}(P) - \gamma$$

and

$$\hat{v} < \mathbb{E}[\hat{v}] + \gamma - \frac{1}{2N} < \text{var}(P) + \gamma$$

we have

$$\Pr(\hat{v} \in (\text{var}(P) - \gamma, \text{var}(P) + \gamma)) > 95\%$$

as required.

3.2 Confidence Interval

Calculating confidence interval functions for $\mathbb{E}[P]$ is far easier than $\text{var}(P)$, so we split them into separate sections.

3.2.1 Mean

We have that

$$u = \hat{\mu}_1 \sim \mathcal{N}\left(\mathbb{E}[P], \frac{m_2 - m_1^2}{Nn^2}\right).$$

Assume we wish to know u within some region with a certain probability i.e.

$$\Pr(u \in (\mathbb{E}[P] - \gamma, \mathbb{E}[P] + \gamma) | N, n) = 1 - \epsilon.$$

Given $\epsilon \in [0, 1]$ and $\gamma > 0$, we wish to solve the above equation for N and n . Well assuming as in the limit that u follows a normal distribution, then we have

$$\Phi\left(\frac{\gamma n \sqrt{N}}{\sqrt{m_2 - m_1^2}}\right) - \Phi\left(\frac{-\gamma n \sqrt{N}}{\sqrt{m_2 - m_1^2}}\right) = 1 - \epsilon$$

where Φ is the cdf of a standard normal distribution. Using the symmetry of the normal distribution about 0,

$$\Phi\left(\frac{\gamma n \sqrt{N}}{\sqrt{m_2 - m_1^2}}\right) = 1 - \epsilon/2.$$

Alternatively we probably just want to make sure that we are at least 95% sure we are *within* the given confidence interval, given both parameters N and n can vary i.e.

$$\Phi\left(\frac{\gamma n \sqrt{N}}{\sqrt{m_2 - m_1^2}}\right) > 1 - \epsilon/2. \tag{1}$$

3.2.2 Variance

In order to find confidence intervals using v we note that it is actually just the sample variance of Z_i plus a term that goes to zero as $n \rightarrow \infty$. We proceed as follows

$$\begin{aligned} v &= \frac{n\hat{\mu}_2 - \hat{\mu}_1 - (n-1)\hat{\mu}_1^2}{n-1} \\ &= \frac{n}{n-1}(\hat{\mu}_2 - \hat{\mu}_1^2) + \frac{1}{n-1}(\hat{\mu}_1^2 - \hat{\mu}_1) \\ &= \frac{n}{n-1} \left[\frac{1}{N} \sum_{i=1}^N \frac{Z_i^2}{n^2} - \left(\frac{1}{N} \sum_{i=1}^N \frac{Z_i}{n} \right)^2 \right] + \frac{\hat{\mu}_1^2 - \hat{\mu}_1}{n-1} \\ &= \frac{N-1}{Nn(n-1)} \left[\frac{N \sum_{i=1}^N Z_i^2 - \left(\sum_{i=1}^N Z_i \right)^2}{N(N-1)} \right] + \frac{\hat{\mu}_1^2 - \hat{\mu}_1}{n-1} \end{aligned}$$

The term in square brackets is simply the sample variance of Z written

$$s^2(Z) = \frac{N \sum_{i=1}^N Z_i^2 - \left(\sum_{i=1}^N Z_i \right)^2}{N(N-1)}.$$

We note when considering the second term that as $\hat{\mu}_1 \in [0, 1]$,

$$0 < \frac{\hat{\mu}_1^2 - \hat{\mu}_1}{n-1} < \frac{1}{4(n-1)}$$

and so as $n, N \rightarrow \infty$, $v \rightarrow \frac{s^2(Z)}{n^2}$. Its a result [?] that asymptotically the sample variance tends to the following

$$s^2(Z) \rightarrow \mathcal{N} \left(\sigma^2(Z), \frac{\mathbb{E}[(Z - \mathbb{E}[Z])^4] - \sigma^4(Z)}{N} \right)$$

where $\sigma(Z) = \sqrt{\mathbb{E}[Z^2] - \mathbb{E}[Z]^2}$ is the standard deviation of Z . So writing using our $\mathbb{E}[Z^k] = m_k$ notation we have

$$v \rightarrow \mathcal{N} \left(\frac{m_2 - m_1^2}{n^2}, \frac{m_4 - 4m_3m_1 + 8m_2m_1^2 - 4m_1^4 - m_2^2}{Nn^4} \right)$$

which gives us the asymptotic distribution we require.

A quick sanity check shows that as $n \rightarrow \infty$,

$$\frac{m_2 - m_1^2}{n^2} = \frac{n\alpha\beta(\alpha + \beta + n)}{n^2(\alpha + \beta)^2(\alpha + \beta + 1)} \rightarrow \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} = \text{var}(P)$$

as we would expect.

Now, assume we wish to know v within some region with a certain probability i.e.

$$\Pr(v \in (\text{var}(P) - \gamma, \text{var}(P) + \gamma) | N, n) = 1 - \epsilon.$$

Given $\epsilon \in [0, 1]$ and $\gamma > 0$, we wish to solve the above equation for N and n . Well assuming as in the limit that v follows a normal distribution, then we have using the symmetry of the normal distribution about 0,

$$\Phi \left(\frac{\gamma n^2 \sqrt{N}}{\sqrt{m_4 - 4m_3m_1 + 8m_2m_1^2 - 4m_1^4 - m_2^2}} \right) = 1 - \epsilon/2.$$

where Φ is the cdf of a standard normal distribution.

Alternatively we probably just want to make sure that we are at least 95% sure we are *within* the given confidence interval, given both parameters N and n can vary i.e.

$$\Phi\left(\frac{\gamma n^2 \sqrt{N}}{\sqrt{m_4 - 4m_3 m_1 + 8m_2 m_1^2 - 4m_1^4 - m_2^2}}\right) > 1 - \epsilon/2. \quad (2)$$

As we mentioned before, it isn't pretty, but the m_k are simply functions of α, β and n .

We can now think of equations (3.2.1) and (2) as giving some constraints on our N and n values and we aim to minimise $N(n + \delta)$ subject to those constraints. We may want to add some further constraints i.e. $N > 1000$ and $n > 500$ to make sure the CLT is taking effect and we don't choose some trivially small solution.

3.3 Example

3.3.1 Mean

Let's again use the case mentioned in the abstract, where we want to know the event to 3 decimal place with *at least* probability 95%. In this case we have

$$\epsilon = 0.05$$

and

$$\gamma = 0.0005.$$

We must also set values for α and β , which we take as

$$\alpha = 0.5$$

and

$$\beta = 0.5.$$

Plugging into our moment equations we get

$$m_1^2 = \frac{n^2}{4}$$

and

$$m_2 = \frac{n(3n+1)}{8}$$

So

$$\begin{aligned} & \frac{0.0005n\sqrt{N}}{(\sqrt{n(3n+1) - 2n^2})/8} > 1.96 \\ \Rightarrow & 8 \cdot 0.0005^2 n^2 N > 1.96^2 (n(3n+1) - 2n^2) \\ \Rightarrow & \frac{8 \cdot 0.0005^2}{1.96^2} n^2 N - n^2 - n > 0 \end{aligned} \quad (3)$$

where we used $\Phi^{-1}(0.975) = 1.96$. Note that we can rearrange and using the fact $n, N > 0$, we get

$$\frac{8 \cdot 0.0005^2}{1.96^2} N - 1 > \frac{1}{n}$$

which means that N must satisfy

$$N > \frac{1.96^2}{8 \cdot 0.0005^2} = 1920800$$

Table 1: Table of N satisfying (3) for different n

n	N
2	2881200
5	2304960
10	2112880
100	1940008
1000	1922720
10000	1920992

Of course if we use near the minimal value of N , it could result in extremely large n values. If instead we use a few different values of n we can get corresponding N values necessary to be within the limits.

Note that despite the fact there isn't that much improvement in simulations as it increases, we expect small n values to require many more simulations to get a decent $\text{var}(P)$ estimate. Note also that the α and β values chosen may not reflect reality (in this case it gives a much larger variance than we would expect). Practically we want to choose values for these that roughly make sense for a given event. The next table shows simulation numbers for different γ, α, β, n values.

Table 2: Table of N satisfying 95% confidence interval for different γ, α, β, n

γ	α	β	n	N
0.0005	0.5	0.5	1000	1922720
0.0005	5	5	1000	352728
0.0005	5	5	100	384160
0.0005	50	50	1000	41839
0.0005	50	50	100	76071
0.005	50	50	100	418

The above values were calculated using `mean_sims.py`. We see that as the values of α and β increase (i.e. $\text{var}(P)$ decreases) the number of simulations N necessary rapidly decreases.

3.3.2 Variance

TODO

4 RESULTS AND DISCUSSION

Reference to Figure 1 on the following page.

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4.1 Subsection

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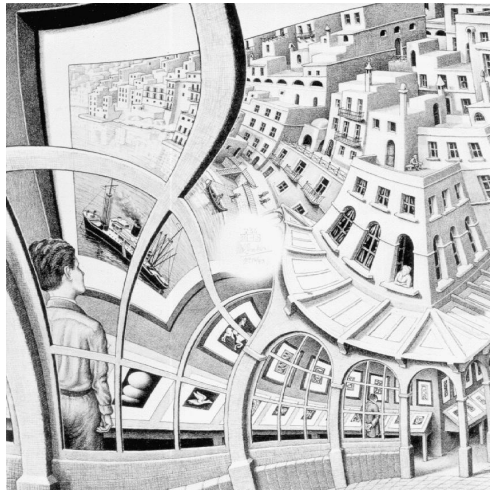


Figure 1: An example of a floating figure (a reproduction from the *Gallery of prints*, M. Escher, from <http://www.mcescher.com/>).

ris. Curabitur malesuada erat sit amet massa. Fusce blandit. Aliquam erat volutpat. Aliquam euismod. Aenean vel lectus. Nunc imperdiet justo nec dolor.

4.1.1 Subsubsection

Etiam euismod. Fusce facilisis lacinia dui. Suspendisse potenti. In mi erat, cursus id, nonummy sed, ullamcorper eget, sapien. Praesent pretium, magna in eleifend egestas, pede pede pretium lorem, quis consectetur tortor sapien facilisis magna. Mauris quis magna varius nulla scelerisque imperdiet. Aliquam non quam. Aliquam porttitor quam a lacus. Praesent vel arcu ut tortor cursus volutpat. In vitae pede quis diam bibendum placerat. Fusce elementum convallis neque. Sed dolor orci, scelerisque ac, dapibus nec, ultricies ut, mi. Duis nec dui quis leo sagittis commodo.

WORD Definition

CONCEPT Explanation

IDEA Text

Etiam euismod. Fusce facilisis lacinia dui. Suspendisse potenti. In mi erat, cursus id, nonummy sed, ullamcorper eget, sapien. Praesent pretium, magna in eleifend egestas, pede pede pretium lorem, quis consectetur tortor sapien facilisis magna. Mauris quis magna varius nulla scelerisque imperdiet. Aliquam non quam. Aliquam porttitor quam a lacus. Praesent vel arcu ut tortor cursus volutpat. In vitae pede quis diam bibendum placerat. Fusce elementum convallis neque. Sed dolor orci, scelerisque ac, dapibus nec, ultricies ut, mi. Duis nec dui quis leo sagittis commodo.

- First item in a list
- Second item in a list
- Third item in a list

4.1.2 Table

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Table 3: Table of Grades

Name		
First name	Last Name	Grade
John	Doe	7.5
Richard	Miles	2

Maecenas urna mi, suscipit in, placerat ut, vestibulum ut, massa. Fusce ultrices nulla et nisl.

Reference to Table 3.

4.2 Figure Composed of Subfigures

Reference the figure composed of multiple subfigures as Figure 2 on the following page. Reference one of the subfigures as Figure 2b on the next page.

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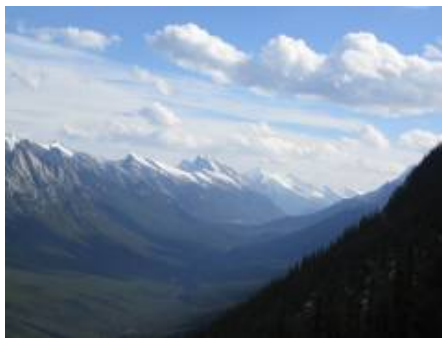
Donec et nisl at wisi luctus bibendum. Nam interdum tellus ac libero. Sed sem justo, laoreet vitae, fringilla at, adipiscing ut, nibh. Maecenas non sem quis tortor eleifend fermentum. Etiam id tortor ac mauris porta vulputate. Integer porta neque vitae massa. Maecenas tempus libero a libero posuere dictum. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Aenean quis mauris sed elit commodo placerat. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Vivamus rhoncus tincidunt libero. Etiam elementum pretium justo. Vivamus est. Morbi a tellus eget pede tristique commodo. Nulla nisl. Vestibulum sed nisl eu sapien cursus rutrum.



(a) A city market.



(b) Forest landscape.



(c) Mountain landscape.



(d) A tile decoration.

Figure 2: A number of pictures with no common theme.