Transforming Probability Spaces

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Table of contents

In Chapter 2 we learned how basic structures, such as metrics and topologies, are transformed when we transform the underlying set. In this chapter we'll learn how measure-theoretic structures are transformed, including probability distributions, expectation values, and probability density functions.

1 Transforming σ-Algebras

We've already seen how to transform subsets Chapter 2. Given two spaces X and Y and any function $f : X \to Y$ we can always push forward subsets in X to subsets in Y by combining the output of each point in the input subset (Figure 1a)

$$f_* : 2^X \to 2^Y$$
$$\mathsf{x} \mapsto f_*\mathsf{x} = \{f(x) \mid x \in \mathsf{x}\}.$$

Similarly we can pull back subsets in Y to subsets in X by combining the preimages of every output point (Figure 1b),

$$f^* : 2^Y \to 2^X$$
$$\mathsf{y} \mapsto \phi^*\mathsf{y} = \{x \in X \mid f(x) \in \mathsf{y}\}.$$
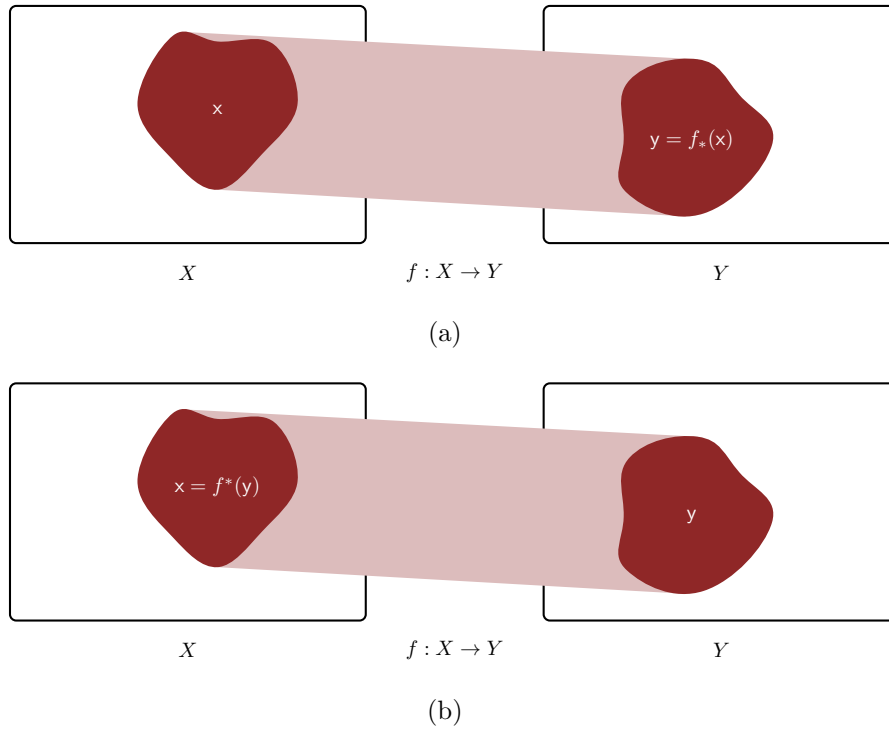

(a)

(b)

Figure 1: Transformations of a set induce transformations of subsets. (a) Subsets of the input space $\mathsf{x} \subset X$ can be pushed forward into subsets of the output space, $f_*(\mathsf{x}) \subset Y$. (b) Similarly subsets of the output space $\mathsf{y} \subset Y$ can be pullsed back into subsets of the input space, $f^*(\mathsf{y}) \subset X$.

There is an asymmetry between these two induced transformations, however, when we consider set operations. Both the pushforward and pullback set maps are compatible with the union operation,

$$f_*(\cup_i \mathsf{x}) = \cup_i f_*(\mathsf{x})$$
$$f^*(\cup_i \mathsf{y}) = \cup_i f^*(\mathsf{y}),$$

but only the pullback map is always compatible with the intersection operation,

$$f^*(\cap_i \mathsf{y}) = \cap_i f^*(\mathsf{y}).$$

In general the intersection of any collection of input subsets pushes forward to a *subset* of the intersection of the individual pushforward subsets (Figure 2).

$$f_*(\cup_i \mathsf{x}) \subseteq \cup_i f_*(\mathsf{x}).$$

This has an immediate consequence for σ-algebras: the pushforward of an intersection of measurable input subsets isn't necessarily a measurable output subset. Consequently a σ-algebra of measurable subsets on X doesn't always push forward into a σ-algebra of measurable subsets on Y.

On the other hand a σ-algebra on Y *does* always pull back to a well-behaved σ-algebra on X. If $\mathcal{Y}$ is a σ-algebra on Y then
$$f^* \mathcal{Y} = \{ f^*(\mathsf{y}) \mid \mathsf{y} \in \mathcal{Y} \}$$
is referred to as the **pullback σ-algebra along** f or the **σ-algebra generated by f\$**.

In order for a function $f : X \to Y$ to preserve the structure of two measurable spaces $(X, \mathcal{X})$ and $(Y, \mathcal{Y})$, every measurable subset $\mathsf{y} \in \mathcal{Y}$ needs to pull back to a measurable subset in $\mathcal{X}$,

$$f^*(\mathsf{y}) \in \mathcal{X},$$

Equivalently f preserves measurable structure only when

$$f^* \mathcal{Y} \subseteq \mathcal{X}.$$

Note that this does not require that *every* measurable subset $\mathsf{x} \in \mathcal{X}$ pushes forward to a measurable subset in $\mathcal{Y}$; we can safely ignore measurable input subsets without compromising the σ-algebra on the output space.

Functions that preserve measurable structure are known as $(\mathcal{X}, \mathcal{Y})$-**measurable functions**. When the σ-algebras on the input and output space are unambiguous this is often shortened to just **measurable functions**.

We've already encountered measurable functions in Chapter 5 when introducing measure-informed integration. A real-valued function $f : X \to \mathbb{R}$ can be integrated on the measure
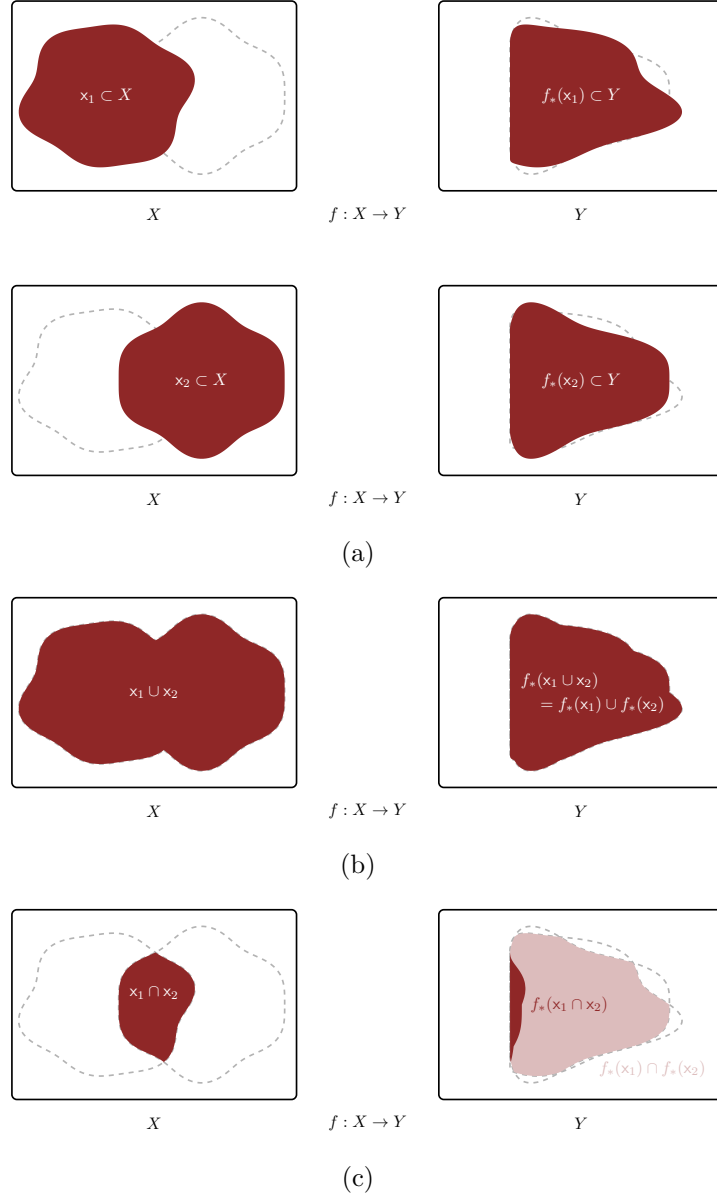
Figure 2: In general (a) subset pushforwards are not consistent with all of the binary set operations. (b) The union of the pushforwards of two input subsets is always the same as the pushforward of the union of the input subsets. (c) On the other hand the intersection of the pushforwards of two input subsets is in generally only a subset of the pushforward of the intersection of the two input subsets. In other words the pushforward operation commutes with the union operator, so that we can apply them in either order and achieve the same result, but the pushforward operation does not commute with the intersection operator. The pullback operation, however, commutes with both the union and intersection operators.

space $(X, \mathcal{X}, \mu)$ if every half-open interval on the output space pulls back to a measurable subset on the input space,

$$f^*((-\infty, x)) \in \mathcal{X}.$$

This condition, however, is equivalent to every subset in the Borel σ-algebra of the real line, $\mathsf{y} \in \mathcal{B}_\mathbb{R}$, pulling back to a measurable subset on the input space,

$$f^*(\mathsf{y}) \in \mathcal{X}.$$

In other words what we referred to as "$\mathcal{X}$-measurable real-valued functions" in Chapter 5 are more formally $(\mathcal{X}, \mathcal{B}_\mathbb{R})$-measurable functions. The former notation takes the Borel σ-algebra on the real line for granted, while the latter makes it more explicit. This is a common shorthand – references to "measurable functions" without any specification almost always imply Borel σ-algebras on the input and output spaces.

Fortunately this shorthand isn't too problematic in practice because we will almost always be working with measures defined over Borel σ-algebras derived from the topological structure of the relevant spaces. Consequently a function $f : X \to Y$ mapping the Borel measurable space $(X, \mathcal{B}_X)$ into the Borel measurable space $(Y, \mathcal{B}_Y)$ might be referred to as $(\mathcal{B}_X, \mathcal{B}Y)$-measurable, **Borel measurable**, or even just "measurable".

Continuous functions that respect the topological structure of the input and outputs spaces are always Borel measurable, but so too are functions that are only piece-wise continuous. Ultimately Borel measurability is a much weaker condition than topological continuity because we can map open subsets in the output space into not only open subsets in the output space, but also closed subsets in the output space and even any subset that we can derive from unions and intersections of open and closed subsets in the input space.

When working with finite-dimensional spaces in practice it is safe to assume that not only all but the most pathological subsets are measurable but also that all but the most pathological functions are measurable. Infinite-dimensional spaces are another matter, but that those spaces will largely be outside of the scope of this book.

2 Transforming Measures

Conveniently the pullback of measurable subsets allows us to pushforward measures from the input space to a compatible measure on the output space. Given a $(\mathcal{X}, \mathcal{Y})$-measurable function $f : X \to Y$ any measure $\mu : \mathcal{X} \to [0, \infty]$ defines a **pushforward measure** by the allocations

$$\begin{aligned} f_*\mu : \mathcal{Y} &\to \mathbb{R}^+ \\ \mathsf{y} &\mapsto f_*\mu(\mathsf{y}) = \mu(f^*(\mathsf{y})). \end{aligned}$$
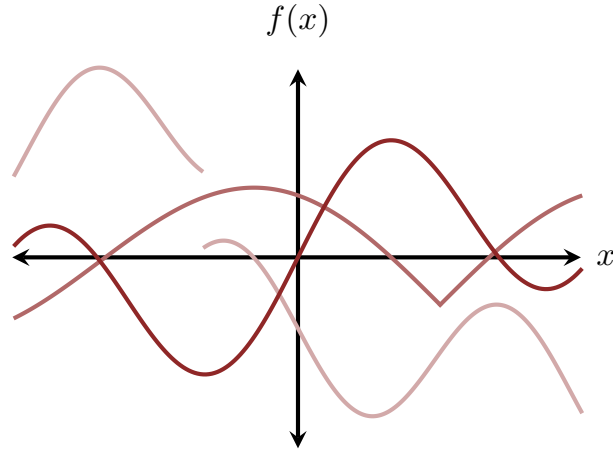
Figure 3: Most of the functions that we encounter in practice are measurable with respect to the standard σ-algebras. For example functions $f : \mathbb{R} \to \mathbb{R}$ that are smooth, non-differentiable but continuous, and even discontinuous at a countable number of points are all $(\mathcal{B}_{\mathbb{R}}, \mathcal{B}_{\mathbb{R}})$-measurable.

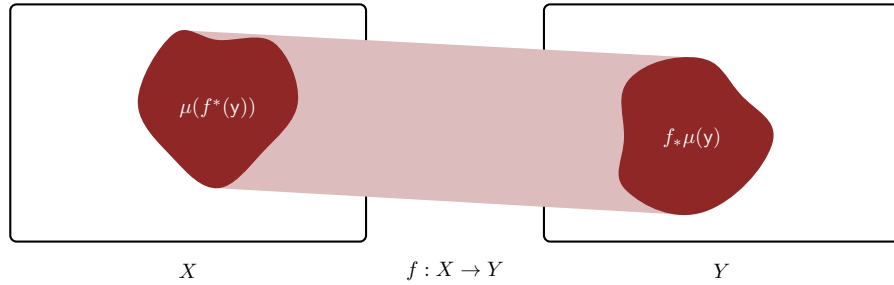Figure 4: Because measurable output subsets pullback to measurable input subsets along measurable functions we can push forward measure allocations. In particular the pushforward measure allocated to the measurable output subset $\mathsf{y} \in \mathcal{Y}$ is given by pulling it back to the input space, $f^*(\mathsf{y}) \in \mathcal{X}$, and then querying the initial measure, $\mu(f^*(\mathsf{y}))$.

In words the pushforward measure allocated to any measurable subset on the output space $y \in \mathcal{Y}$ is computed by pulling the subset back to the input space $f^*(y) \in \mathcal{X}$ and then evaluating the initial measure, $\mu(f^*(y))$ (Figure 4).

The exact interpretation of a pushforward measure will depend on the interpretation of the input measure and the transformation. Consider, for example, a probability distribution π defined on the input space that we interpret as quantifying uncertainty. This probability distribution captures our uncertainty about the *inputs* to a function f while the pushforward probability distribution $f_*\pi$ quantifies the corresponding uncertainty in the *output* of the function. In other words the pushforward transformation *propagates* the initial uncertainty through the deterministic mapping.

At the same time certain functions can endow the corresponding pushforward measures with particular interpretations.

2.1 Pushforward Terminology

Pushforward measures are ubiquitous in applied probability theory, although they are often better known by other names.

For example consider a finite input space X,

$$X = \{\blacksquare, \clubsuit, \bigcirc, \diamondsuit, \triangle, \bowtie\},$$

a finite output space Y,

$$Y = \{\heartsuit, \spadesuit, \ \},$$

and a function $f : X \to Y$ defined by the relations (Figure 5a)

$$f(\blacksquare) = \spadesuit$$
$$f(\clubsuit) = \heartsuit$$
$$f(\bigcirc) =$$
$$f(\diamondsuit) = \spadesuit$$
$$f(\triangle) = \heartsuit$$
$$f(\bowtie) = \spadesuit$$

These relationships between input and output points become particularly well-organized when we arrange the input elements into a table, with each row collecting all of the input elements that map to a particular output element (Figure 5b). Conveniently the pushforward measure allocated to each output atomic subset is then given by summing the input atomic subset allocations in each the corresponding row (Figure 5c, Figure 5c). In other words the pushforward allocations fit nicely into the *margins* of the table.
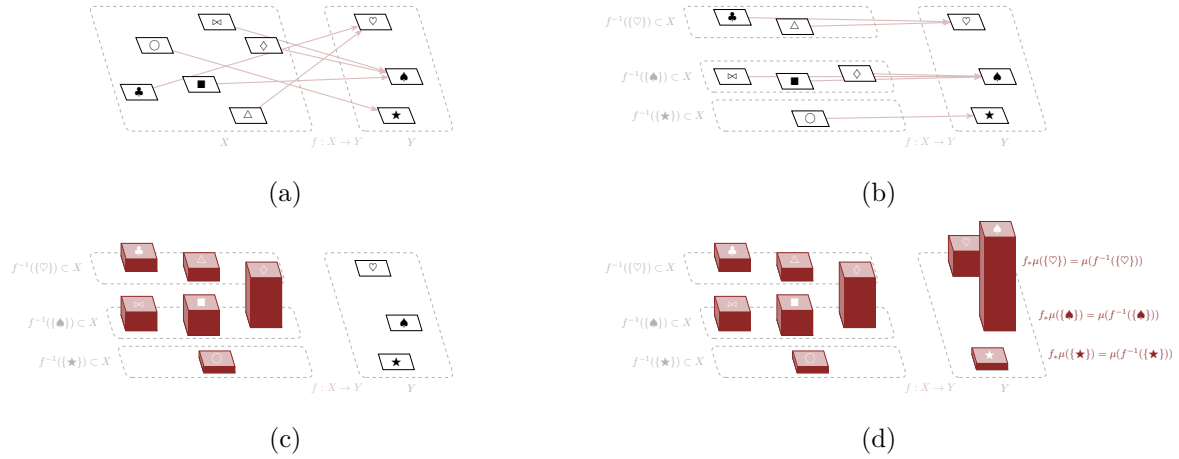
Figure 5: On finite spaces (a) functions $f : X \to Y$ (b) are naturally organized into tables, with each row collecting all of the input points that map to each output point. (c) Given an input measure μ (d) we can compute the pushforward measure allocations by summing the μ allocations in each row and then displaying the results in the margins of the table.

Historically these kinds of graphical organizations motivated the term **marginal measure** to describe pushforward measures, or **marginal probability distribution** in the case of an input probability distribution. Today this terminology is common even when the input and output spaces are not finite, and the tabular representation of functions isn't quite as useful (Figure 6).

Another popular naming convention arises when the output space is a subset of the input space, $Y \subset X$. In this case a function $f : X \to Y$ **projects** the input space onto the output subset (Figure 7). Pushing forward measures along this projection *collapses* the total measure allocated to the input space into the smaller output space.

Consider for example the unit interval interpreted as a subset of a real line,

$$(0, 1) \subset R.$$

One way to squeeze the entire real line into $(0, 1)$ is to apply the **logistic function**,

$$\text{logistic} : \mathbb{R} \to (0, 1)$$

$$x \mapsto \frac{1}{1 + \exp(-x)}.$$

The logistic function preserves topological structure, pushing open intervals in $\mathbb{R}$ forward into open intervals in $(0, 1)$,

$$\text{logistic}_*(\,(x_1, x_2)\,) = (\,\text{logistic}(x_1), \text{logistic}(x_2)\,).$$

8

{#fig-level-sets}

(a)   (b)
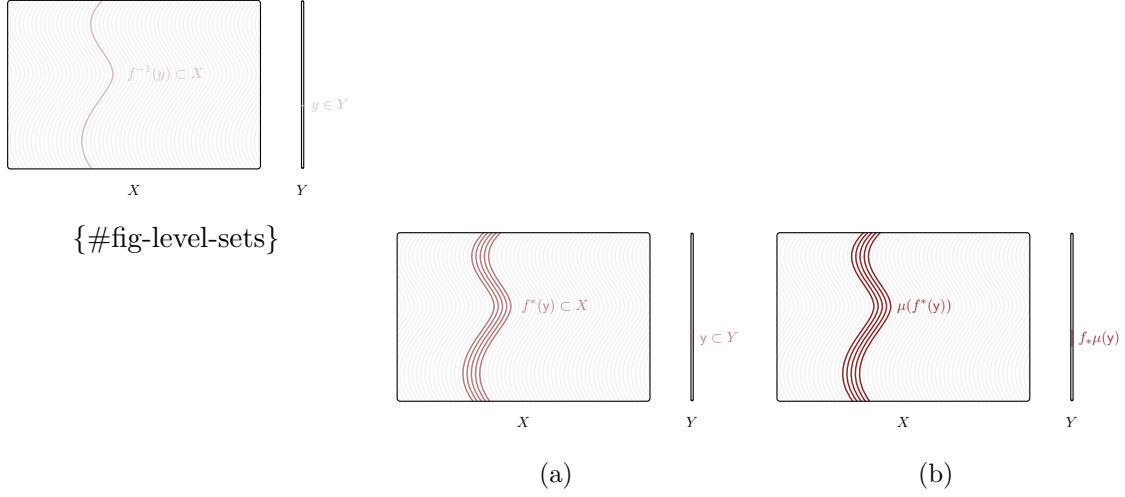
Figure 6: When working on general spaces the tabular organization of a function $f : X \to Y$ generalizes to (a) collections of level sets $f^{-1}(y) \subset X$, one for each output point $y \in Y$. (b) The pullback of any output subset is the union of these level sets and (c) the pushforward measure allocated to any output subset is effectively the sum of the measures allocated to the relevant level sets. These pushforward allocations can then be informally collected into the "margins".

At the same time open intervals in $(0, 1)$ are pulled back into open intervals in $\mathbb{R}$,

$$\text{logistic}^* ((y_1, y_2)) = (\text{logistic}^{-1}(y_1), \text{logistic}^{-1}(y_2)).$$

Consequently the logistic function is Borel measurable.

When pushing forward measures along the logistic function the measure allocated to any open interval is squeezed into a narrower interval,

$$\mu_* ((y_1, y_2)) = \mu(\text{logistic}^* ((y_1, y_2)))$$
$$= \mu((\text{logistic}^{-1}(y_1), \text{logistic}^{-1}(y_2))).$$

2.2 Lossy Pushforward Measures

We can always push measures forward along measurable functions, but in general we cannot pull them back. This asymmetry arises because the pushforward operation can *lose informa-tion*.
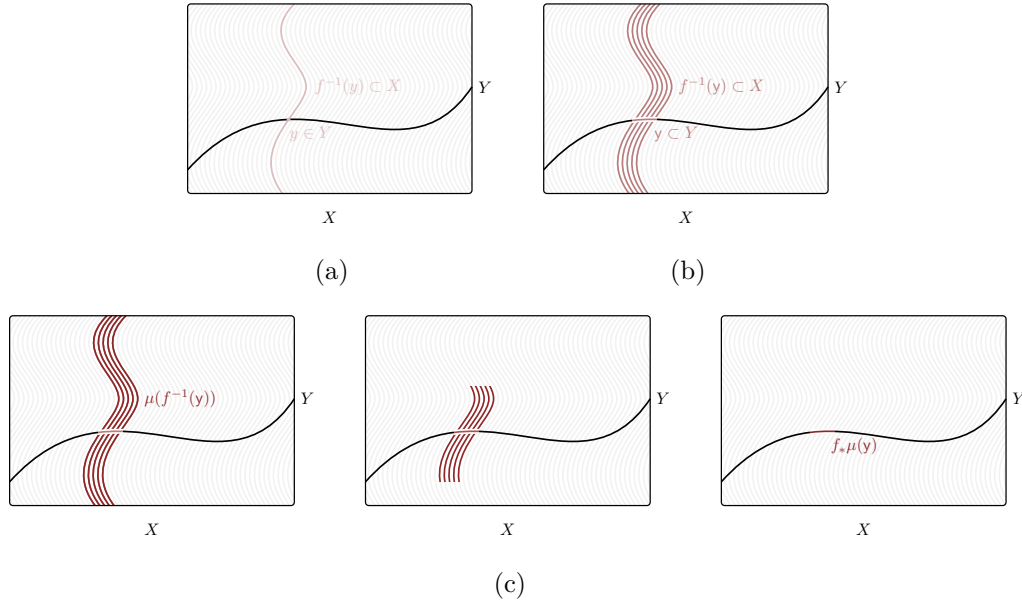
Figure 7: When a function $f : X \to Y$ maps an input space into a subset of itself, $Y \subset X$, then pushforward measures can be interpreted as projections of the initial measure. (a) In this case each level set $f^{-1}(y)$ is anchored to a point $y \in X$ and (b) the pullback of an output subset is anchored to the points in that subset. (c) The pushforward measure collapsed the measure allocated to each level set down to the corresopnding anchor point.

Figure 8: The logistic function squeeze an entire real line into the unit interval. When we push an input measure forward along the logistic function the measure allocated to an input intervals is squeezed into a narrow interval.

10

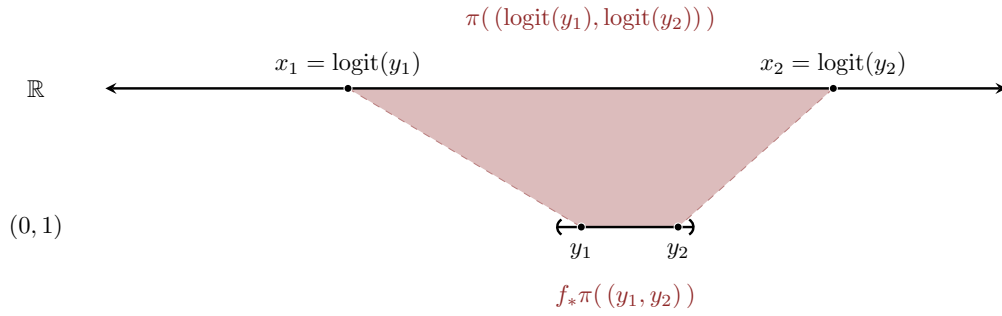Consider the function between finite spaces that we introduced in Section 2.1. A measure μ on the input space defines the pushforward atomic allocation

$$
\begin{aligned}
f_*\mu(\{\heartsuit\}) &= \mu(f^*(\heartsuit)) \\
&= \mu(\{\clubsuit, \triangle\}) \\
&= \mu(\{\clubsuit\}) + \mu(\{\triangle\}).
\end{aligned}
$$

Because input elements $\clubsuit$ and $\triangle$ map to the same output element their atomic allocations are combined into a single pushforward atomic allocation.

If we are given only the pushforward allocation $f_*\mu(\{\heartsuit\})$ then we will not have enough information to fully recover the initial allocations $\mu(\{\triangle\})$ and $\mu(\{\triangle\})$. We can constrain their sum,

$$ f_*\mu(\{\heartsuit\}) = \mu(\{\clubsuit\}) + \mu(\{\triangle\}), $$

but there are infinitely many input measures consistent with such a constraint.

For a more sophisticated example let's investigate a function that maps a real line into integers by rounding each real number to the next largest integer,

$$
\begin{aligned}
f &: \mathbb{R} \to \mathbb{Z} \\
x &\mapsto \lceil x \rceil.
\end{aligned}
$$

This function collapses every point in the half-open interval $(n-1, n]$ to the integer n so that the atomic subsets on the output space pull back to those input intervals (Figure 9),

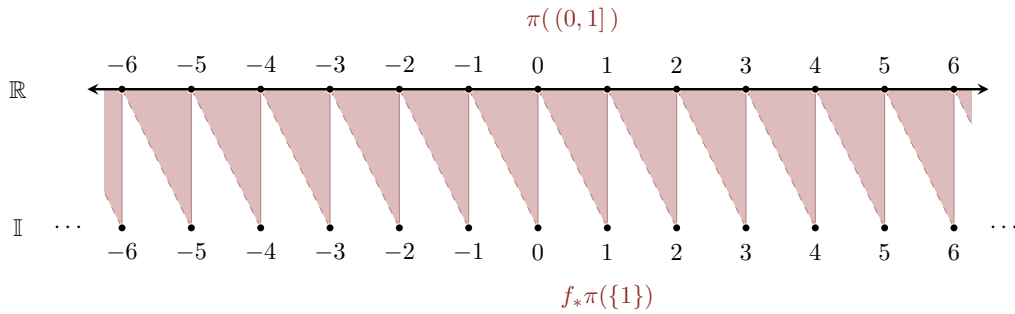$$ f^*(\{n\}) = (n-1, n]. $$

Figure 9: Rounding real numbers to the next-largest integer defines a map from a real line to the integers. Input measure allocated to the half-open intervals $(n-1, n]$ projects down to the corresponding integer n.

Along f the Lebesgue measure on the real line pushes forward to a measure on the integers with the atomic allocations

$$
\begin{aligned}
f_*\lambda(\{n\}) &= \lambda(f^*(\{n\})) \\
&= \lambda(\,(n, n-1]\,) \\
&= n - (n-1) \\
&= 1.
\end{aligned}
$$

In other words the pushforward of the Lebesgue measure along this rounding map is just the counting measure!

The counting measure on the output space, however, does not provide any information about how to distribute the atomic allocation $\chi(\{n\}) = 1$ across the entire pullback subset $(n-1, n]$. Instead there are an infinite numbers of ways that the measure $\chi(\{n\}) = 1$ could be consistently reallocated across $(n-1, n]$ and we have no criteria for preferring one over another.

2.3 Lossless Pushforward Measures

Because most pushforward measures lose information about the initial allocations the exceptional measures that preserve information are particulary notable.

As we saw in Section 1 pushforward sets do not generally respect the intersection set operator, preventing us from pushing forward σ-algebras from the input space to the output space. Pushing sets forward along injective functions, however, does respect the intersection operator. Consequently we can always push forward σ-algebras along injective functions.

When working with measurable spaces that are already equipped with σ-algebras, $(X, \mathcal{X})$ and $(Y, \mathcal{Y})$ any injective function $f : X \to Y$ that both pulls back measurable output subsets to measurable input subsets,

$$
f^*(\mathsf{y}) \subset \mathcal{X}.
$$

and pushes forward measurable input subsets to measurable output subsets,

$$
f_*(\mathsf{x}) \subset \mathcal{Y}.
$$

is said to be $\{\mathcal{X}, \mathcal{Y}\}$-**bimeasurable**, or simply **bimeasurable** when the σ-algebras are unambiguous.

Because the pushforward and pullback maps along injective functions always satisfy

$$
f^* \circ f_* = I
$$

we also have

$$
f^*(\mathcal{Y}) = \mathcal{X}.
$$

In other words the σ-algebra generated by a bimeasurable function is just the initial input σ-algebra.

As with measurable functions, bimeasurable functions allow us to push forward any measure on the input space $\mu : \mathcal{X} \to [0, \infty]$ to a corresponding measure on the output space $\mu_* : \mathcal{Y} \to [0, \infty]$ with the allocations

$$\mu_*(\mathsf{y}) = \mu(\, f^*(\mathsf{y})\,).$$

Bimeasurable functions also allow us to pull back any measure $\nu : \mathcal{Y} \to [0, \infty]$ on the output space to a corresponding measure $\nu^* : \mathcal{X} \to [0, \infty]$ on the input space with the allocations

$$\nu^*(\mathsf{x}) = \nu(\, f_*(\mathsf{x})\,).$$

Importantly these operations are consistent with each other. Pulling back a pushforward measure along a bimeasurable function recovers the initial measure allocations,

$$\begin{aligned} f^*\mu_*(\mathsf{x}) &= \mu^*(\, f_*(\mathsf{x})\,) \\ &= \mu(\, f^* \circ f_*(\mathsf{x})\,) \\ &= \mu(\mathsf{x}). \end{aligned}$$

In other words we are always able to completely reconstruct the initial measure from the pushforward allocations alone. Bimeasurable functions don't loose any information about the initial allocations!

Two measure spaces $(X, \mathcal{X}, \mu)$ and $(Y, \mathcal{Y}, \nu)$ that are related by a bimeasurable function $f : X \to Y$ provide equivalent measure-theoretic information,

$$\begin{aligned} f_*\mu &= \nu \\ f^*\nu &= \mu. \end{aligned}$$

Because they quantify the same information they can be interpreted as different mathematical *representations* of a common, abstract measure system.

For example every permutation of a finite set is not only injective but also preserves the discrete σ-algebra. Consequently every permutation of a finite set is bimeasurable, transforming any discrete measure into another, equivalent discrete measure. In practice this means that we are free to choose the permutation that yields the most convenient organization of the underlying set without having to worry about compromising the information encoded in the original space!

Similarly every continuous bijection between two real lines is bimeasurable with respect to the Borel σ-algebras. Continuous bijections then allow us to transform a measure over a rigid real line into any a measure on another rigid real line without losing information. Equivalently these maps allow us to transform a measure over any parameterization of a flexible real line into a measure over any other parameterization of that flexible space without losing any resolution of the system. This gives us the freedom to choose the most convenient units or coordinate system in practice without having to worry about affecting the measure behavior.

3 Transforming Measure-Informed Integrals

Once we know how to transform subset allocations we can, at least in theory, define integrals with respect to a pushforward measure on the output space and relate them to integrals with respect to the initial measure on the input space. Fortunately that relationship ends up being relatively straightforward.

Given a function $\phi : X \to Y$ any real-valued function on the output space $f : Y \to \mathbb{R}$ pulls back to a real-valued function on the input space $\phi^* f : X \to \mathbb{R}$ by composition,

$$\phi^* f(x) = f \circ \phi(x) = f(\phi(x)).$$

Additionally if $\phi : X \to \mathbb{R}$ is a $(\mathcal{X}, \mathcal{Y})$-measurable function and $f : Y \to \mathbb{R}$ is a $(\mathcal{Y}, \mathbb{B}_{\mathbb{R}})$-measurable function then $\phi^* f = f \circ \phi$ will always be a $(\mathcal{X}, \mathbb{B}_{\mathbb{R}})$-measurable function. In other words integrands on the output space always pullback to integrands on the input space along measurable transformations.

Given an initial measure μ and its pushforward $\phi_* \mu$ we can use these two integrands to define two measure-informed integrals,

$$\mathbb{I}_\mu[\phi^* f]$$

on the input space and

$$\mathbb{I}_{\phi_* \mu}[f]$$

on the output space. Conveniently these measure-informed integrals are always equal,

$$\mathbb{I}_\mu[\phi^* f] = \mathbb{I}_{\phi_* \mu}[f].$$

When we're working with probability distributions this becomes a relationship between equivalent expectation values,

$$\mathbb{E}_\pi[\phi^* f] = \mathbb{E}_{\phi^* \pi}[f].$$

Critically this relationship means that we don't actually have to explicitly construct a pushforward measure in practice. So long as we know how to compute integrals with respect to μ then we can compute integrals with respect to $\phi_* \mu$ by pulling back the output integrand,

$$\phi^* f = f \circ \phi.$$

Fortunately this is often straightforward to implement in practice.

While we're on the topic of measure-informed integration, notice that we have two ways for a measure space $(X, \mathcal{X}, \mu)$ to consume a $(\mathcal{X}, \mathcal{B}_{\mathbb{R}})$-measurable function $f : X \to \mathbb{R}$. So long as f is μ-integrable we can integrate f with respect to μ to give the single real number $\mathbb{I}_\mu[f] \in \mathbb{R}$. On the other hand we can also push μ forward along f to construct an entire measure $f_* \mu$ over the possible output values!

The mean of the pushforward measure $f_*\mu$ is given by

$$
\begin{aligned}
\mathbb{M}_{f^*\mu} &= \mathbb{I}_{f^*\mu}[\iota] \\
&= \mathbb{I}_\mu[\iota \circ f] \\
&= \mathbb{I}_\mu[f].
\end{aligned}
$$

In other words the mu-informed integral of f is always equal to the mean of the corresponding pushforward measure!

Because of this concurrence the μ-informed integral of a function is sometimes referred to as "the mean of f". Similarly the μ-informed integral of

$$
\begin{aligned}
\mathbb{I}_{f^*\mu}[(\iota - \mathbb{M}_{f^*\mu})^2] &= \mathbb{I}_\mu[(\iota \circ f - \mathbb{M}_{f^*\mu})^2] \\
&= \mathbb{I}_\mu[(f - \mathbb{M}_{f^*\mu})^2]
\end{aligned}
$$

is sometimes referred to as "the variance of f".

Personally I try to avoid this terminologies because I find that they facilitate confusion between the two operations. I do not, however, shy away from using certain mu-informed integrals to quantify the properties of a pushforward measure $f_*\mu$. Indeed this is an incredibly powerful tool in practice and one that we discuss more thoroughly in Section 5.

4 Transforming Probability Density Functions

In practice we rarely, if ever, define probability distributions with subset allocations but rather rely on probability density functions with respect to convenient reference measures. To transform probability distributions in this applied context we will need to know how to push forward probability density functions along measurable transformations.

4.1 Directly Transforming Probability Density Functions

When an initial probability distribution π and reference measure ν are fixed the transformation properties of the corresponding probability density function is straightforward to construct for bijective functions.

On the input space we can define the probability density function

$$
\frac{\mathrm{d}\pi}{\mathrm{d}\nu} : X \to \mathbb{R}^+.
$$

At the same time given a $(\mathcal{X}, \mathcal{Y})$-measurable function $f : X \to Y$ we can push forward both π and ν to measures on the output space and construct the probability density function between them,

$$
\frac{\mathrm{d}f_*\pi}{\mathrm{d}f_*\nu} : Y \to \mathbb{R}^+.
$$

Because we're using a consistent reference measure these two functions are related by composition,

$$\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x) \overset{\nu}{=} \frac{\mathrm{d}f_*\pi}{\mathrm{d}f_*\nu} \circ f(x).$$

In other words the output probability density function $\mathrm{d}f_*\pi/\mathrm{d}f_*\nu$ pulls back to the input probability density function $\mathrm{d}\pi/\mathrm{d}\nu$.

When f is a bijection we can use its inverse to construct an output probability density function from an input probability density function,

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}f_*\nu}(y) \overset{f_*\nu}{=} \frac{\mathrm{d}\pi}{\mathrm{d}\nu} \circ f^{-1}(y).$$

In a practice, however, the pushforward of the initial reference measure $f_*\nu$ might not actually be the most convenient reference measure on the output space. For example a uniform measure over the input space will not generally push forward to a uniform measure over the output space. If we want to construct probability density functions on the output space relative to a *different* reference measure λ then the relevant probability density function we need is no longer

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}f_*\nu} : Y \to \mathbb{R}^+.$$

but rather

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda} : Y \to \mathbb{R}^+.$$

Fortunately we can still relate this output probability density function to the initial probability density function with the Radon-Nikodym chain rule. If $f_*\nu$ is absolutely continuous with respect to λ then we can expand the desired output probability density function into

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y) \overset{\lambda}{=} \frac{\mathrm{d}f_*\pi}{\mathrm{d}f_*\nu}(y) \cdot \frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y).$$

When f is measurable *and* bijective then we can derive the first contribution from the initial probability density function and the function inverse,

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y) \overset{\lambda}{=} \frac{\mathrm{d}\pi}{\mathrm{d}\nu} \circ f^{-1}(y) \cdot \frac{\mathrm{d}f_*\nu}{\mathrm{d}\lambda}(y).$$

The second term in this transformation formula,

$$\frac{\mathrm{d}f_*\nu}{\mathrm{d}\lambda}(y),$$

quantifies how *warped* the pushforward reference measure $f_*\nu$ is relative to the desired reference measure λ. When

$$\frac{\mathrm{d}f_*\nu}{\mathrm{d}\lambda}(y) \overset{\lambda}{=} 1$$

the two reference measures are equivalent and the transformation rule reduces to our initial calculation.

Unfortunately this warping contribution is often difficult to compute, limiting how often we can applying the transformation formula directly. To compute it in practice we usually need to consider the transformation properties of measure-informed integrals,

$$\mathbb{I}_\nu[g \circ f] = \mathbb{I}_{f_*\nu}[g]$$

$$\mathbb{I}_\nu[g \circ f] = \mathbb{I}_\lambda\left[\frac{\mathrm{d}f_*\nu}{\mathrm{d}\lambda} \cdot g\right].$$

If we can relate ν-informed integration on the input space to λ-informed integration out the output space then this relationship may allow us to compute the warping factor $\mathrm{d}f_*\nu/\mathrm{d}\lambda$.

Constructing pushforward probability density functions along non-bijective functions is much more complicated. Ultimately we need to relate π-informed integration on the input space to λ-informed integration on the output space,

$$\mathbb{E}_\pi[g \circ f] = \mathbb{I}_{f_*\pi}[g]$$

$$\mathbb{I}_\nu\left[\frac{\mathrm{d}\pi}{\mathrm{d}\nu} \cdot g \circ f\right] = \mathbb{I}_\lambda\left[\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda} \cdot g\right]$$

$$\int_X \nu(\mathrm{d}x)\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x) \cdot g(f(x)) = \int_Y \lambda(\mathrm{d}y)\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y) \cdot g(y).$$

If $f : X \to Y$ is surjective then, at least conceptually, we might be able to implement the ν-informed integral over the input space *iteratively*, first integrating over the the individual level sets of f before aggregating those intermediate results,

$$\int_X \nu(\mathrm{d}x)\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x) \cdot g(f(x)) = \int_Y \lambda(\mathrm{d}y)\left[\int_{f^{-1}(y)} \kappa_y(\mathrm{d}z)\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x(y,z))\right] \cdot g(y).$$

In this case we would have

$$\int_Y \lambda(\mathrm{d}y)\left[\int_{f^{-1}(y)} \kappa_y(\mathrm{d}z)\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x(y,z))\right] \cdot g(y) = \int_Y \lambda(\mathrm{d}y)\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y) \cdot g(y)$$

or

$$\frac{\mathrm{d}f_*\pi}{\mathrm{d}\lambda}(y) = \int_{f^{-1}(y)} \kappa_y(\mathrm{d}z)\frac{\mathrm{d}\pi}{\mathrm{d}\nu}(x(y,z)).$$

To be clear this is entirely a casual argument. Formalizing it, in particular defining exactly what the measures across the level sets $\kappa_y(\mathrm{d}z)$ need to be to ensure consistent results is a subtle mathematical problem. Conveniently we'll tackle this exact problem when we introduce *conditional* probability theory in the next chapter.

4.2 Transforming Probability Mass Functions

When X and Y are both discrete measurable spaces then probability density functions with respect to the respective counting measures reduce to probability mass functions. In this case we can conveniently compute the transformation properties directly by applying the transformation rule for measure-informed integrals to counting measures and indicator functions,

$$\mathbb{I}_{\chi_X}[I_{\{y'\}} \circ f] = \mathbb{I}_{f_*\chi_X}[I_{\{y'\}}].$$

On the left-hand side we can take advantage of the fact that integration with respect to a counting measure reduces to discrete summation,

$$\mathbb{I}_{\chi_X}[I_{\{y'\}} \circ f] = \mathbb{I}_{\chi_X}\left[I_{\{y'\}} \circ f\right]$$
$$= \sum_{x \in X} I_{\{y'\}}(f(x)).$$

When $f : X \to Y$ is bijective then there will be one, and only one, input point $x \in X$ with $f(x) = y'$ and

$$\mathbb{I}_{\chi_X}[I_{\{y'\}} \circ f] = \sum_{x \in X} I_{\{y'\}}(f(x)) = 1.$$

Moving over to the right-hand side we have to convert to the output counting measure before summing,

$$\mathbb{I}_{f_*\chi_X}[I_{\{y'\}}] = \mathbb{I}_{\chi_Y}\left[\frac{\mathrm{d}f_*\chi_X}{\mathrm{d}\chi_Y} \cdot I_{\{y'\}}\right]$$
$$= \sum_{y \in Y} \frac{\mathrm{d}f_*\chi_X}{\mathrm{d}\chi_Y}(y) \cdot I_{\{y'\}}(y)$$
$$= \frac{\mathrm{d}f_*\chi_X}{\mathrm{d}\chi_Y}(y').$$

Putting the two results together gives

$$\mathbb{I}_{\chi_X}[I_{\{y'\}} \circ f] = \mathbb{I}_{f_*\chi_X}[I_{\{y'\}}]$$
$$1 = \frac{\mathrm{d}f_*\chi_X}{\mathrm{d}\chi_Y}(y')$$

for any $y' \in Y$. In other words counting measures on discrete spaces always map to other counting measures under bijections; no two counting measures will ever appear warped relative to each other so long as the input and output spaces have the same number of elements.

Substituting this into the transformation rule for probability density functions under bijections gives an explicit transformation rule for probability mass functions $p : X \to [0,1]$,

$$
\begin{aligned}
f_* p(y) &= \frac{\mathrm{d} f_* \pi}{\mathrm{d} \chi_Y}(y) \\
&= \frac{\mathrm{d} \pi}{\mathrm{d} \chi_X} \circ f^{-1}(y) \cdot \frac{\mathrm{d} f_* \chi_X}{\mathrm{d} \chi_Y}(y) \\
&= \frac{\mathrm{d} \pi}{\mathrm{d} \chi_X} \circ f^{-1}(y) \cdot 1 \\
&= \frac{\mathrm{d} \pi}{\mathrm{d} \chi_X} \circ f^{-1}(y) \\
&= p \circ f^{-1}(y).
\end{aligned}
$$

More generally for any expectand $g : Y \to \mathbb{R}$ we should have

$$
\mathbb{E}_\pi[g \circ \phi] = \mathbb{E}_{f_* \pi}[g]
$$
$$
\mathbb{I}_{\chi_X}\left[\frac{\mathrm{d} \pi}{\mathrm{d} \chi_X} \cdot g \circ f \right] = \mathbb{I}_{\chi_Y}\left[\frac{\mathrm{d} f_* \pi}{\mathrm{d} \chi_Y} \cdot g \right]
$$
$$
\mathbb{I}_{\chi_X}[p \cdot g \circ f] = \mathbb{I}_{\chi_Y}[f_* p \cdot g]
$$
$$
\sum_{x \in X} p(x) \cdot g(f(x)) = \sum_{y \in Y} f_* p(y) \cdot g(y).
$$

Because the input space is discrete we can readily organize the summation on the left-hand side any way we want. In particular we can always add up the contributions from the elements in each level set $f^{-1}(y)$ first and then combine all of those contributions,

$$
\sum_{x \in X} = \sum_{y \in Y} \sum_{x \in f^{-1}(y)}.
$$

Using this organization gives

$$
\sum_{x \in X} p(x) \cdot g(f(x)) = \sum_{y \in Y} f_* p(y) \cdot g(y)
$$
$$
\sum_{y \in Y} \sum_{x \in f^{-1}(y)} p(x) \cdot g(f(x)) = \sum_{y \in Y} f_* p(y) \cdot g(y)
$$
$$
\sum_{y \in Y} \sum_{x \in f^{-1}(y)} p(x) \cdot g(y) = \sum_{y \in Y} f_* p(y) \cdot g(y)
$$
$$
\sum_{y \in Y} \left[\sum_{x \in f^{-1}(y)} p(x) \right] \cdot g(y) = \sum_{y \in Y} f_* p(y) \cdot g(y).
$$

This is true for any expectand g if and only if

$$
f_* p(y) = \sum_{x \in f^{-1}(y)} p(x).
$$

When $f : X \to Y$ is a bijection each level set contains a single input element,

$$f_* p(y) = \sum_{x \in f^{-1}(y)} p(x)$$
$$= p(f^{-1}(y))$$
$$= p \circ f^{-1}(y),$$

consistent with what we derived above.

To put this all into context let's consider a product space built up from N binary component spaces,

$$X = \{0, 1\}^N,$$

and a probability distribution specified by the probability mass function

$$p(x) = p(x_1, \ldots, x_N)$$
$$= \prod_{n=1}^N p(x_n)$$
$$= \prod_{n=1}^N \theta^{x_n} (1 - \theta)^{1 - x_n}$$
$$= \theta^{\sum_{n=1}^N x_n} (1 - \theta)^{\sum_{n=1}^N (1 - x_n)}$$
$$= \theta^{\sum_{n=1}^N x_n} (1 - \theta)^{\sum_{n=1}^N 1 - \sum_{n=1}^N x_n}$$
$$= \theta^{\sum_{n=1}^N x_n} (1 - \theta)^{N - \sum_{n=1}^N x_n}$$

for some $\theta \in (0, 1)$.

Moreover, let's say that we want to push this probability mass function forward along the function

$$s : \{0, 1\}^N \quad \to [0, N]$$
$$(x_1, \ldots, x_N) \mapsto \ = \sum_{n=1}^N x_n.$$

The level sets of this function, $s^{-1}(y)$ are given by all of the product elements with n component elements equalling one and $N - y$ component elements equalling zero. Because there are

$$\binom{N}{y} = \frac{N!}{y! \, (N - y)!}$$

different ways that we can set y distinct components to one, there are that many elements in the level set $s^{-1}(y)$.

The probability mass function that defines the pushforward probability distribution over the sum of ones is given by applying the general transformation rule,

$$
\begin{aligned}
s_* p(y) &= \sum_{x \in s^{-1}(y)} p(x) \\
&= \sum_{x \in s^{-1}(y)} \theta^{\sum_{n=1}^{N} x_n} (1-\theta)^{N - \sum_{n=1}^{N} x_n} \\
&= \sum_{x \in s^{-1}(y)} \theta^y (1-\theta)^{N-y} \\
&= \left[\sum_{x \in s^{-1}(y)} 1 \right] \theta^y (1-\theta)^{N-y} \\
&= \binom{N}{y} \theta^y (1-\theta)^{N-y}.
\end{aligned}
$$

This is known as a **Binomial probability mass function** for its dependence on the binomial coefficient.

4.3 Transforming Lebesgue Probability Density Functions

Unfortunately when working on real spaces we can no longer work with summation. Technically the warping factor $\mathrm{d}f_* \lambda_X / \mathrm{d}\lambda_Y$ can be derived from a sophisticated theoretical analysis – see for example Theorem 2.47 in Folland (1999) – but here we will work it out from the more familiar properties of Riemann integration.

4.3.1 The Jacobian Correction

Let's say that $X = \mathbb{R}^N$ and $Y = \mathbb{R}^N$ are two rigid, N-dimensional real spaces related by the bijective transformation $f : X \to Y$. Moreover let λ_X and λ_Y be the Lebesgue measures on X and Y, respectively.

In this case the transformation rule for measure-informed integrals,

$$
\mathbb{I}_{\lambda_X}[g \circ f] = \mathbb{I}_{\lambda_Y}\left[\frac{\mathrm{d}f_* \lambda_X}{\mathrm{d}\lambda_Y} \cdot g \right],
$$

reduces to a relationship between Riemann integrals,

$$
\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N y \, \frac{\mathrm{d}f_* \lambda_X}{\mathrm{d}\lambda_Y}(y) \, g(y),
$$

at least for sufficiently nice integrands $g : Y \to \mathbb{R}$.

This closely matches the infamous change-of-variables property from calculus (Apostol (1969)). For a transformation $h : Y \to X$ and integrand $q : X \to \mathbb{R}$ we have

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, q(x) = \int_{\mathbb{R}^N} \mathrm{d}^N y \, |\det \mathbf{J}_h(y)| \, q(h(y)),$$

where $|\det \mathbf{J}_h(x)|$ is the absolute value of the determinant of the **Jacobian matrix** with elements

$$J_{h,ij}(y) = \frac{\partial h_i}{\partial y_j}(y).$$

Taking $h = f^{-1}$ and $q = g \circ f$ this becomes

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N x \, |\det \mathbf{J}_{f^{-1}}(y)| \, g(f(f^{-1}(y)))$$

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N x \, |\det \mathbf{J}_{f^{-1}}(y)| \, g(y).$$

Conveniently this simplifies a bit due to the fact that the Jacobian matrix of f^{-1} at y is equal to the matrix inverse of the Jacobian matrix of f at $x = f^{-1}(y)$,

$$\mathbf{J}_{f^{-1}}(y) = \mathbf{J}_f^{-1}(f^{-1}(y)).$$

In particular this relationship implies that

$$\det \mathbf{J}_{f^{-1}}(y) = \frac{1}{\det \mathbf{J}_f(f^{-1}(y))}$$

and consequently

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N x \, \frac{1}{|\det \mathbf{J}_f(f^{-1}(y))|} \, g(y).$$

To review: for any sufficiently well-behaved integrand $g : Y \to \mathbb{R}$ we have both

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N y \, \frac{\mathrm{d} f_* \lambda_X}{\mathrm{d} \lambda_Y}(y) \, g(y)$$

and

$$\int_{\mathbb{R}^N} \mathrm{d}^N x \, g(f(x)) = \int_{\mathbb{R}^N} \mathrm{d}^N x \, \frac{1}{|\det \mathbf{J}_f(f^{-1}(y))|} \, g(y).$$

Comparing the two equations the warping factor must be given by (Figure 10)

$$\frac{\mathrm{d} f_* \lambda_X}{\mathrm{d} \lambda_Y}(y) \overset{\lambda_Y}{=} \frac{1}{|\det \mathbf{J}_f(f^{-1}(y))|}.$$

Because the warping factor reduces to a Jacobian determinant it is also known as a **Jacobian correction**.
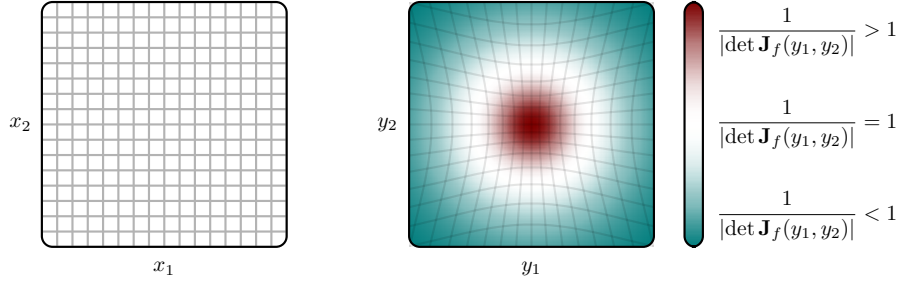
Figure 10: The reciprocal of the absolute value of the Jacobian determinant function, $1/\det \mathbf{J}_f(f^{-1}(y))$ quantifies how warped the input Lebesgue measure appears relative to the output Lebesgue measure. If the warping factor is smaller than one then the input volumes appear to expand and if the warping factor is larger than one then the input volumes appear to contract.

A nearly universal convention in applied probability theory ignores the fact that this relationship has to hold for only λ_Y-almost all $y \in Y$ and just takes the warping factor to be

$$\frac{\mathrm{d}f_*\lambda_X}{\mathrm{d}\lambda_Y}(y) = \frac{1}{|\det \mathbf{J}_f(f^{-1}(y))|}.$$

for all output points $y \in Y$.

With this convention the transformation rule for Lebesgue probability density functions along bijective transformations becomes (Figure 11, Figure 12)

$$f_*p(y) \stackrel{\lambda_Y}{=} p(f^{-1}(y)) \frac{\mathrm{d}f_*\lambda_X}{\mathrm{d}\lambda_Y}(y)$$

$$\stackrel{\lambda_Y}{=} p(f^{-1}(y)) \frac{1}{|\det \mathbf{J}_f(f^{-1}(y))|}.$$

All of this careful work ensures that probability allocations derived from the pushforward Lebesgue probability density function are consistent with the probability allocations derived from the initial Lebesgue probability density function. In particular we always have (Figure 13)

$$\pi(\mathsf{x}) = f_*\pi(f_*\mathsf{x})$$

$$\mathbb{E}_\pi[I_\mathsf{x}] = \mathbb{E}_{f_*\pi}[I_{f_*\mathsf{x}}]$$

$$\mathbb{I}_{\lambda_X}[p \cdot I_\mathsf{x}] = \mathbb{E}_{\lambda_Y}[f_*p \cdot I_{f_*\mathsf{x}}]$$

$$\int_{\mathbb{R}^N} \mathrm{d}^N x\, p(x) \cdot I_\mathsf{x}(x) = \int_{\mathbb{R}^N} \mathrm{d}^N y\, f_*p(y) \cdot I_{f_*\mathsf{x}}(y)$$

$$\int_\mathsf{x} \mathrm{d}^N x\, p(x) \cdot I_\mathsf{x}(x) = \int_{f_*\mathsf{x}} \mathrm{d}^N y\, f_*p(y).$$
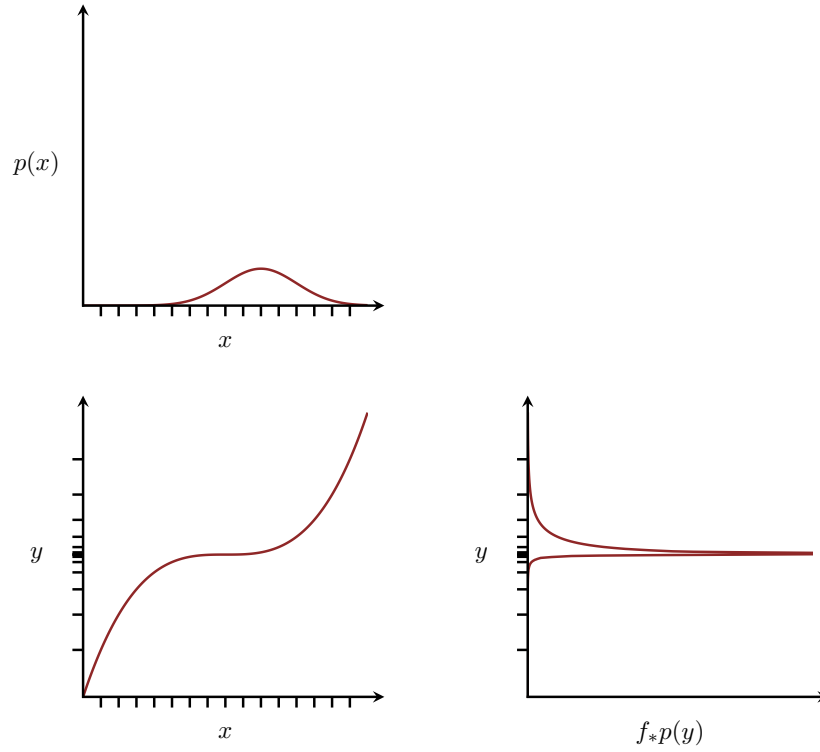
23

Figure 11: In general bijective functions from one real space to another warp both probability distributions and reference Lebesgue measures. In order to transform Lebesgue probability density functions we have to account for both of these changes.
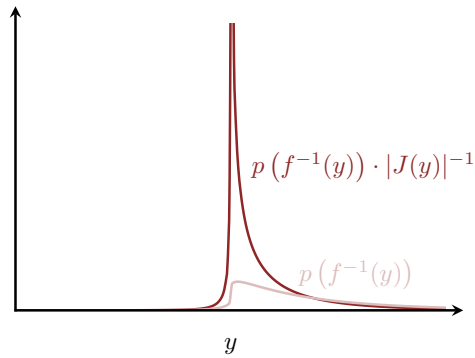

Figure 12: Ignoring the Jacobian correction that accounts for the change in Lebesgue reference measure results in erroneous pushforward probability density functions. This error affects not only the normalization of the pushforward probability density function but also its shape.

$\pi(\mathsf{x})$ $\pi_*(f_*(\mathsf{x}))$

x_2 y_2

$f_*(\mathsf{x})$

x_1 y_1
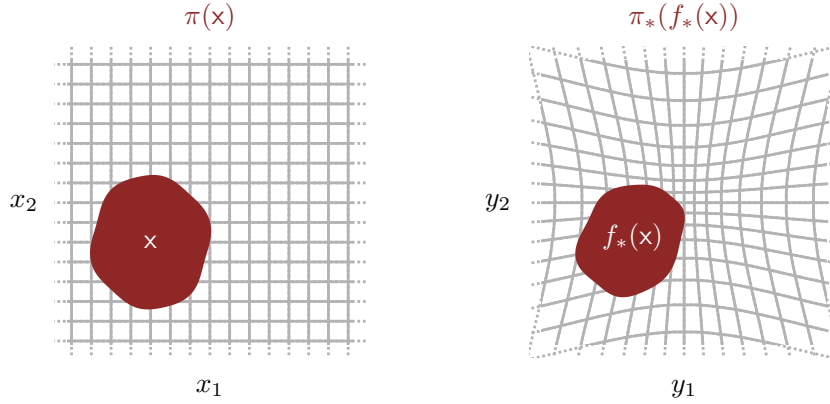
Figure 13: The proper transformation rule for Lebesgue probability density functions allows us to consistently compute probability allocations on the input space and the output space.

When applying the transformation rule for probability density functions in practice the most common mistake is forgetting the Jacobian correction entirely. The second most common error is forgetting to take the reciprocal of the Jacobian determinant, mistakingly using

$$f_* p(y) \overset{\lambda_Y}{=} p(f^{-1}(y)) \left| \det \mathbf{J}_f(f^{-1}(y)) \right|.$$

To avoid this mistake I rely on a mneumonic to help me remember the proper orientation of the Jacobian determinant. I start with the informal integral relationship,

$$\int \mathrm{d}y \, f_* p(y) = \int \mathrm{d}x \, p(x),$$

drop the integral signs,

$$\mathrm{d}y \, f_* p(y) = \mathrm{d}x \, p(x),$$

and then very informally divide by the differentials,

$$\mathrm{d}y \, f_* p(y) = \mathrm{d}x \, p(x)$$

$$f_* p(y) = p(x) \, \frac{\mathrm{d}x}{\mathrm{d}y}(x)$$

$$f_* p(y) = p(x(y)) \, \frac{1}{\frac{\mathrm{d}y}{\mathrm{d}x}(x)}$$

$$f_* p(y) = p(x) \, \frac{1}{|mathrmdet \, \mathbf{J}_f(x)|}$$

$$f_* p(y) = p(f^{-1}(y)) \, \frac{1}{|mathrmdet \, \mathbf{J}_f(f^{-1}(y))|}.$$

This is by no means a formal calculation – each step is extremely mathematically sloppy – but the result is quick to derive and gives the correct orientation of the Jacobian correction.

Is there anything we can do about non-bijective functions? We might be tempted to utilize the Dirac delta function to iterate expectation values on the input space as

$$\int_X \mathrm{d}x\, \pi(x)\, g(f(x)) = \int_Y \mathrm{d}y \left[\int_{f^{-1}(y)} \mathrm{d}x\, \pi(x) \right] g(y)$$

$$= \int_Y \mathrm{d}y \left[\int_X \mathrm{d}x\, \pi(x) \delta(f(x) - y) \right] g(y)$$

so that

$$f_* \pi(y) \overset{\lambda_Y}{=} \int_X \mathrm{d}x\, \pi(x) \delta(f(x) - y),$$

and indeed this notation is not uncommon in some applied fields. Unfortunately it's not clear how we can actually implement these integrals in practice. In the next chapter we'll see how we can formalize this strategy using *conditional* expectation values to implement the integrals over each level set.

4.3.2 Examples

After all of that discussion let's put these results in practice with a few concrete examples.

4.3.2.1 Translating and Scaling

Consider a probability distribution over a rigid real line, or a fixed parameterization of a flexible real line, specified by a normal probability density function

$$\mathrm{normal}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right).$$

A translation function maps each point in the input real line to a translated point in the output real line,

$$t_\delta : \mathbb{R} \to \mathbb{R}$$
$$x \mapsto x + \delta.$$

This function is a bijection, with the inverse function translating points in the opposite direction,

$$t_\delta^{-1} : \mathbb{R} \to \mathbb{R}$$
$$y \mapsto y - \delta.$$

Because the translation operator maps a one-dimensional space into another one-dimensional space its Jacobian determinant reduces to a single derivative function,

$$
\begin{aligned}
\det \mathbf{J}_{t_\delta}(x) &= \frac{\mathrm{d}t_\delta}{\mathrm{d}x}(x) \\
&= \frac{\mathrm{d}}{\mathrm{d}x}(x + \delta) \\
&= 1.
\end{aligned}
$$

Consequently the Jacobian correction is particularly straightforward,

$$
\frac{1}{|\det \mathbf{J}_{t_\delta}(t_\delta^{-1}(y))|} = \frac{1}{|1|} = 1.
$$

With the Jacobian correction in hand the pushforward of a normal density function along a translation operator becomes

$$
\begin{aligned}
(t_\delta)_* \mathrm{normal}(y; \mu, \sigma) &= \mathrm{normal}(t_\delta^{-1}(y); \mu, \sigma)) \cdot \frac{1}{|\det \mathbf{J}_{t_\delta}(t_\delta^{-1}(y))|} \\
&= \mathrm{normal}(y - \delta; \mu, \sigma) \cdot 1 \\
&= \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{y - \delta - \mu}{\sigma}\right)^2\right) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{y - (\mu + \delta)}{\sigma}\right)^2\right) \\
&= \mathrm{normal}(y; \mu + \delta, \sigma).
\end{aligned}
$$

In other words pushing a normal probability density function along a translation operator results in another normal probability density function, only one with a shifted location parameter (Figure 14).

A scale function maps each point in the input space to a scaled point in the output space,

$$
\begin{aligned}
s_\phi &: \mathbb{R} \to \mathbb{R} \\
x &\mapsto \phi \cdot x
\end{aligned}
$$

for any $\phi > 0$. This is also a bijection, with the inverse function scaling points by the reciprocal of ϕ,

$$
\begin{aligned}
s_\phi^{-1} &: \mathbb{R} \to \mathbb{R} \\
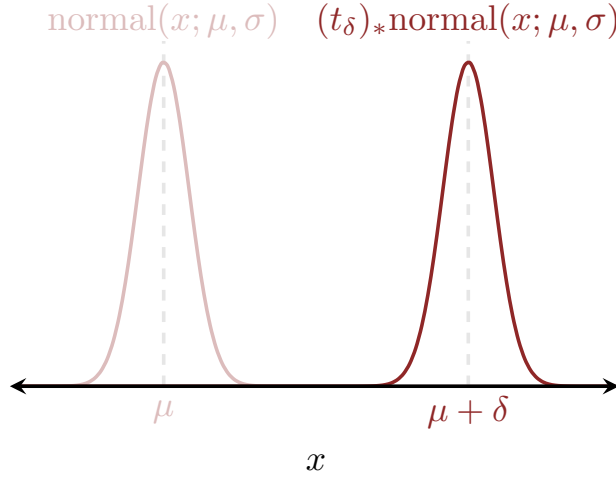y &\mapsto \frac{y}{\phi}.
\end{aligned}
$$

$$\text{normal}(x; \mu, \sigma) \qquad (t_\delta)_* \text{normal}(x; \mu, \sigma)$$

Figure 14: A translation operator t_δ shifts a normal probability density function with location parameter μ to another normal probability density function with location parameter $\mu + \delta$. The scale parameter σ is unaffected.

The Jacobian determinant once again reduces to just a single derivative function,

$$
\begin{aligned}
\det \mathbf{J}_{s_\phi}(x) &= \frac{\mathrm{d}s_\phi}{\mathrm{d}x}(x) \\
&= \frac{\mathrm{d}}{\mathrm{d}x}(\phi \cdot x) \\
&= \phi
\end{aligned}
$$

In this case the Jacobian correction is slightly more complicated,

$$
\frac{1}{|\det \mathbf{J}_{s_\phi}(s_\phi^{-1}(y))|} = \frac{1}{|\phi|} = \frac{1}{\phi}.
$$

The pushforward of a normal density function along a scale function is then given by

$$(s_\phi)_* \text{normal}(y; \mu, \sigma) = \text{normal}(s_\phi^{-1}(y); \mu, \sigma)) \cdot \frac{1}{|\det \mathbf{J}_{s_\phi}(s_\phi^{-1}(y))|}$$

$$= \text{normal}(y/\phi; \mu, \sigma) \frac{1}{\phi}$$

$$= \frac{1}{\sqrt{2\pi}\sigma} \cdot \frac{1}{\phi} \exp\left(-\frac{1}{2}\left(\frac{y/\phi - \mu}{\sigma}\right)^2\right)$$

$$= \frac{1}{\sqrt{2\pi}(\phi \cdot \sigma)} \exp\left(-\frac{1}{2}\left(\frac{y - \phi \cdot \mu}{\phi \cdot \sigma}\right)^2\right)$$

$$= \text{normal}(y; \phi \cdot \mu, \phi \cdot \sigma).$$

As before pushing a normal probability density function along a scale operator results in another normal probability density function. In this case, however, both the location and scale parameters are affected (Figure 15).
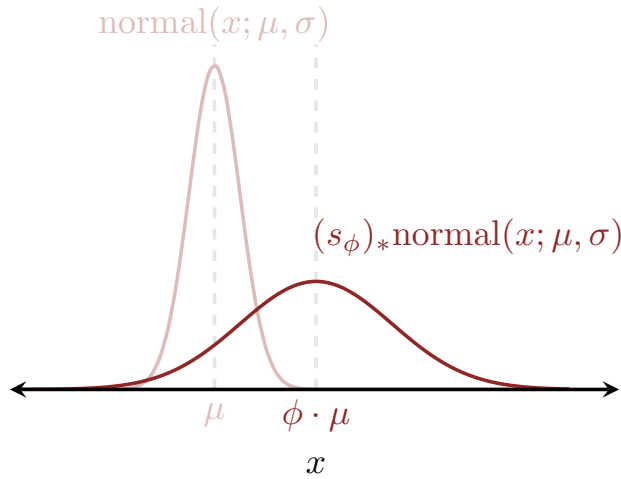
Figure 15: A scale operator s_ϕ transforms a normal probability density function with location parameter μ and scale parameter σ into normal probability density function with the inflated location parameter $\phi \cdot \mu$ and inflated scale parameter $\phi \cdot \sigma$.

These two operations can also be combined into a single function that first scales and then translates,

$$st_{\delta,\phi} = t_\delta \circ s_\phi$$

with

$$st_{\delta,\phi} : \mathbb{R} \to \mathbb{R}$$
$$x \mapsto \phi \cdot x + \delta.$$

This composition defines another bijection, with the inverse function scaling points by the reciprocal of the scaling parameter before translating in the opposite direction,

$$st_{\delta,\phi}^{-1} = s_\phi^{-1} \circ t_\delta^{-1}$$

with

$$st_{\delta,\phi}^{-1} : \mathbb{R} \to \mathbb{R}$$
$$y \mapsto \frac{y - \delta}{\phi}.$$

The Jacobian determinant for this composition is

$$\det \mathbf{J}_{st_{\delta,\phi}}(x) = \frac{\mathrm{d}st_{\delta,\phi}}{\mathrm{d}x}(x)$$
$$= \frac{\mathrm{d}}{\mathrm{d}x}(\phi \cdot x + \delta)$$
$$= \phi,$$

with the Jacobian correction becoming

$$\frac{1}{|\det \mathbf{J}_{st_{\delta,\phi}}(st_{\delta,\phi}^{-1}(y))|} = \frac{1}{|\phi|} = \frac{1}{\phi}.$$

Pushing forward a normal probability density function along this composite function then gives

$$(st_{\delta,\phi})_*\mathrm{normal}(y; \mu, \sigma) = \mathrm{normal}(st_{\delta,\phi}^{-1}(y); \mu, \sigma) \cdot \frac{1}{|\det \mathbf{J}_{st_{\delta,\phi}}(s_\phi^{-1}(y))|}$$
$$= \mathrm{normal}((y - \delta)/\phi; \mu, \sigma) \cdot (1/\phi)$$
$$= \frac{1}{\sqrt{2\pi}\sigma} \frac{1}{\phi} \exp\left(-\frac{1}{2} \left(\frac{(y - \delta)/\phi - \mu}{\sigma} \right)^2 \right)$$
$$= \frac{1}{\sqrt{2\pi}(\phi \cdot \sigma)} \exp\left(-\frac{1}{2} \left(\frac{y - (\phi \cdot \mu + \delta)}{\phi \cdot \sigma} \right)^2 \right)$$
$$= \mathrm{normal}(y; \phi \cdot \mu + \delta, \phi \cdot \sigma).$$

No matter how we scale and translate an ambient real line, a normal probability density function will always map into another normal probability density function.

In fact if we start with the **unit normal probability density function**

$$\text{unit-normal}(x) = \text{normal}(x; 0, 1),$$

then the pushforward probability density function along the scale-translation function becomes

$$(st_{\delta,\phi})_*\text{unit-normal}(y) = \text{normal}(y; \delta, \phi).$$

Consequently we can generate *every* normal probability density function as a suitable transformation of an initial, unit normal probability density function. Because of this the normal family of probability density functions is known as a **location-scale** family.

4.3.2.2 Squeezing A Real Line Into An Interval

For a more sophisticated example let's look at the logistic function that we introduced in Section 2.1,

$$\text{logistic} : \mathbb{R} \to (0, 1)$$

$$x \mapsto \frac{1}{1 + \exp(-x)}.$$

The logistic function is bijective and its inverse function is known as the **logit function**,

$$\text{logit} : (0, 1) \to \mathbb{R}$$

$$y \quad \mapsto \log \frac{y}{1 - y}.$$

Because this is a one-dimensional transformation the Jacobian determinant reduces to a single derivative function,

$$
\begin{aligned}
\det \mathbf{J}_{\text{logistic}}(x) &= \frac{\text{dlogistic}}{\text{d}x}(x) \\
&= \frac{\text{d}}{\text{d}x}\left(\frac{1}{1 + \exp(-x)}\right) \\
&= -\frac{\exp(-x)}{(1 + \exp(-x))^2} \\
&= -\frac{1}{1 + \exp(-x)}\left(1 - \frac{1}{1 + \exp(-x)}\right) \\
&= -\text{logistic}(x)\left(1 - \text{logistic}(x)\right).
\end{aligned}
$$

The Jacobian correction then becomes

$$
\begin{aligned}
\frac{1}{|\det \mathbf{J}_{\text{logistic}}(\text{logit}(y))|} &= \frac{1}{|-\text{logistic}(\text{logit}(y))\left(1 - \text{logistic}(\text{logit}(y))\right)|} \\
&= \frac{1}{\text{logistic}(\text{logit}(y))\left(1 - \text{logistic}(\text{logit}(y))\right)} \\
&= \frac{1}{y\left(1 - y\right)}.
\end{aligned}
$$

31

The pushforward of a normal density function along the logistic function is now given by (Figure 16)

$$\text{logistic}_*\text{normal}(y; \mu, \sigma) = \text{normal}(\text{logit}(y); \mu, \sigma) \cdot \frac{1}{|\det \mathbf{J}_{\text{logistic}}(\text{logit}(y))|}$$

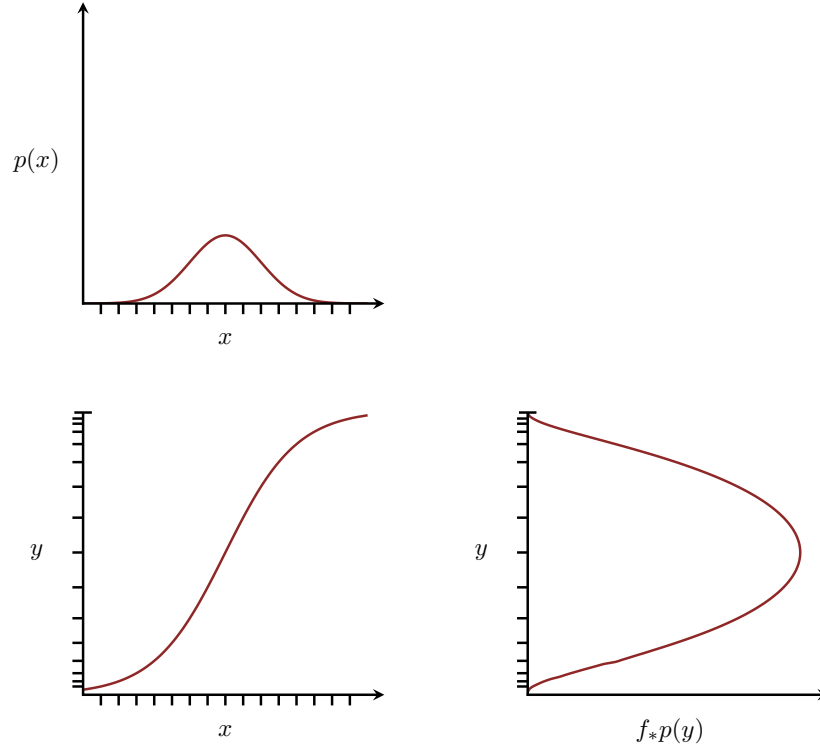$$= \text{normal}(\text{logit}(y); \mu, \sigma)\frac{1}{y(1-y)}.$$

Figure 16: The logistic function squeezes a real line into a unit interval, transforming Lebesgue probability density functions over all real numbers into a Lebesgue probability density function over real numbers $0 < y < 1$.

5 Characterizing One-Dimensional Pushforward Probability Distributions

Probability distributions on high-dimensional spaces are overwhemlming objects that are difficult to study directly. In particular we cannot convey the entirety of a high-dimensional probability distribution in a single visualization. We can, however, push a high-dimensional

probability distribution forward to many one-dimensional probability distributions that can be visualized (Figure 17), not unlike a carpenter checking if a piece of wood is warped by staring down each edge one at a time.
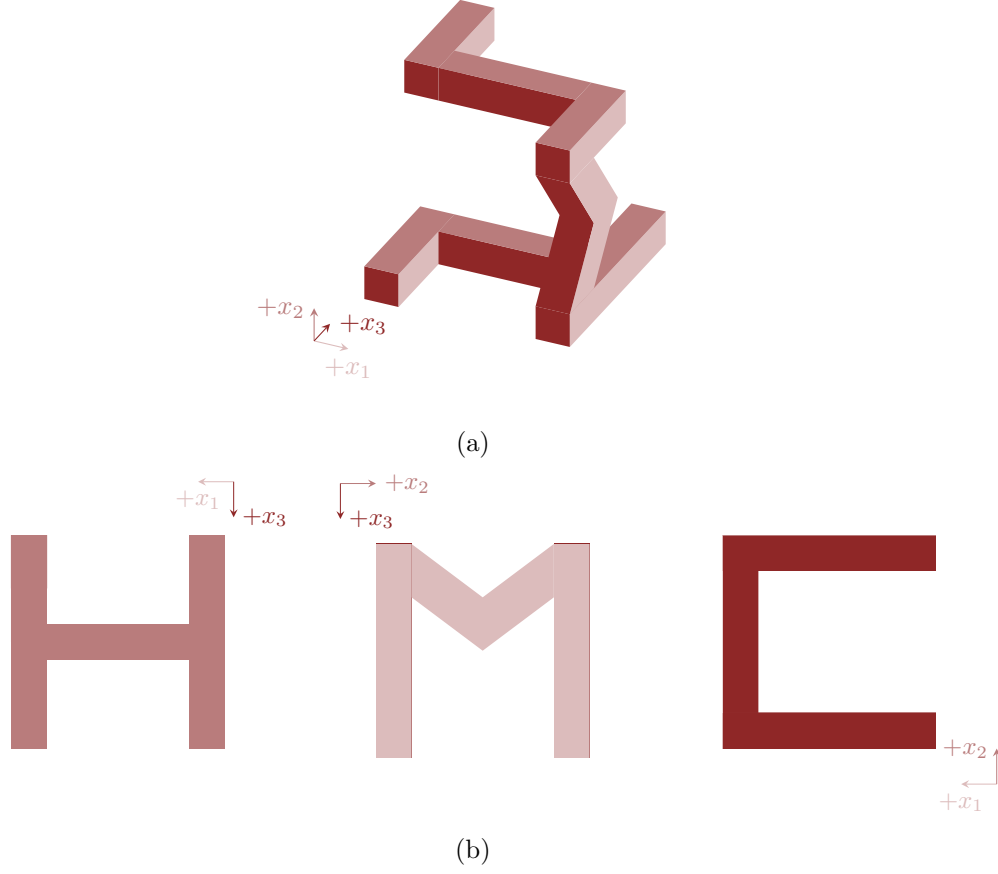

(a)

(b)

Figure 17: In general (a) High-dimensional mathematical objects, such probability distributions over high-dimensional spaces, are difficult to interpret directly. (b) Summary functions map high-dimensional objects to low-dimensional objects, isolating behaviors that can be not only easier to digest but also straightforward to visualize.

More formally given a probability space $(X, \mathcal{X}, \pi)$ and a collection of $(\mathcal{X} - \mathcal{B}_{\mathbb{R}})$-measurable functions

$$f_n : X \to \mathbb{R}$$

we can construct a collection of one-dimensional pushforward probability distributions

$$(f_n)_* \pi.$$

Each of these pushforward probability distributions summarizes a different aspect of π; the

more interpretable the outputs of the function f_n are the more interpretable that summary will be.

In order to implementing these probabilistic summaries in practice, however, we need to be able to characterize the pushforward probability distributions. Pushforward probability density functions would be particularly convenient for visualization (Figure 18), but at this point we don't know how to actually compute them yet for non-bijective summary functions. Unfortunately in the next chapter we'll see that the necessary operations are often infeasible in practice.
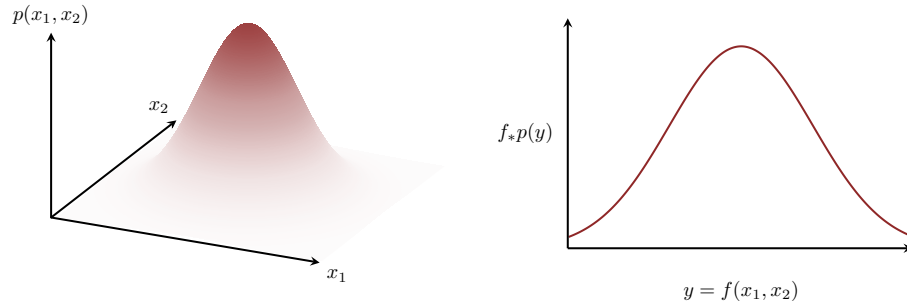
Figure 18: A pushforward probability density functions are particularly useful for visualizing pushforward behavior extracted from a high-dimensional probability distribution, but they often infeasible to construct in practice.

Fortunately in Chapter Five we learned about multiple ways to characterize one-dimensional probability distributions using only expectation values. Moreover if we can compute expectation values on the initial, high-dimensional ambient space then we can use the pullback of expectation values,

$$\mathbb{E}_{f_*\pi}[g] = \mathbb{E}_\pi[g \circ f].$$

to implement these characterizations in practice.

For example in Section 3 we saw that the moments of one-dimensional pushforward distributions can be evaluated as expectation values over the initial space. In particular we can compute the mean and variance of the pushfoward probability distribution $(f_n)_*\pi$ can be evaluated with the expectation values

$$\mathbb{M}_{(f_n)_*\pi} = \mathbb{E}_\pi[f_n]$$

and

$$\mathbb{V}_{f^*\mu} = \mathbb{E}_{(f_n)_*\pi}[(f - \mathbb{m}_{(f_n)_*\pi})^2],$$

respectively. That is, of course, provided that both expectands are integrable.

We can also use expectation values to evaluate pushforward interval probabilities,

$$(f_n)_* \pi(\, (y_1, y_2] \,) = \mathbb{E}_{(f_n)_* \pi}[I_{(y_1, y_2]}]$$
$$= \mathbb{E}_{\pi}[I_{(y_1, y_2]} \circ f_n].$$

These pushforward interval probabilities then allow us to construct histogram representations of each pushforward probability distribution (Figure 19). The narrower the pushforward intervals we use the more these histograms convey the same information that a pushforward probability density function would, especially when we scale the bin probabilities by the interval lengths as we discussed in Chapter Six, Section 4.4.
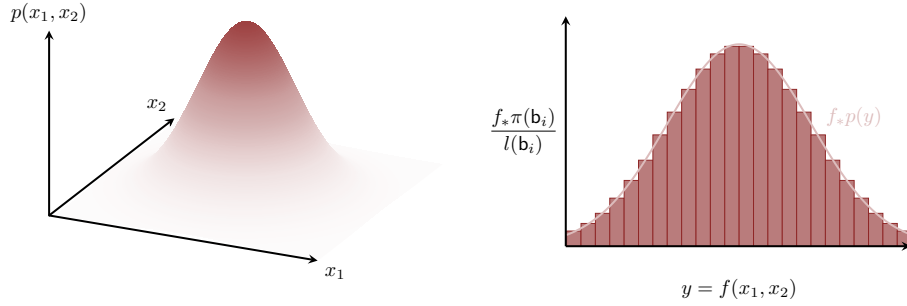
Figure 19: Pushforward histograms visualize similar information as pushforward probability density functions, especially when the binning is narrow, but are much easier to construct.

In theory we can also use pushforward interval probabilities to construct the cumulative distribution functions for a given pushforward probability distribution by computing

$$P_{f_* \pi}(y) = (f_n)_* \pi(\, (-\infty, y] \,)$$
$$= \mathbb{E}_{\pi}[I_{(-\infty, y]} \circ f_n]$$

for each $y \in \mathbb{R}$. Unfortunately completely characterizing a pushforward cumulative distribution function in this way would require an infinite number of expectation value calculations while typical computational budgets afford for only a finite number. Consequently in practice we have to be content with *approximating* pushforward cumulative distribution functions (Figure 20).

Lastly we can often characterize one-dimensional pushforward probability distribution with nested pushforward quantile intervals (Figure 21). While we typically won't be able to compute pushforward quantiles exactly, we can construct reasonable approximations to the p-th quantile by iteratively searching possible values $q_p \in \mathbb{R}$ until

$$|(f_n)_* \pi(\, (-\infty, q_p] \,) - p| = |\mathbb{E}_{\pi}[I_{(-\infty, y]} \circ f_n] - p|$$
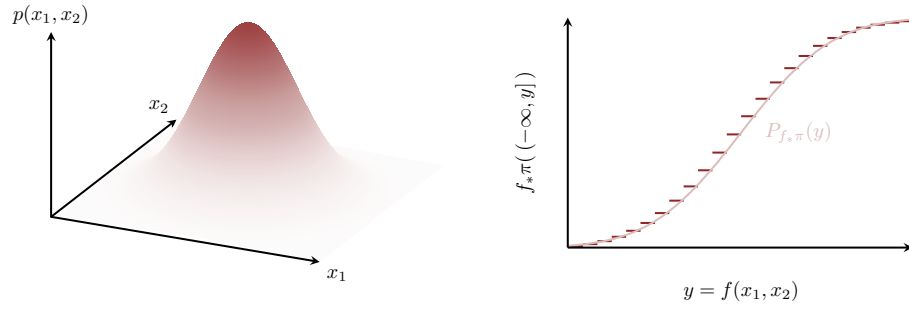
Figure 20: Aggregating bin probabilities also allows us to approximately visualize a pushforward cumualtive distribution function.
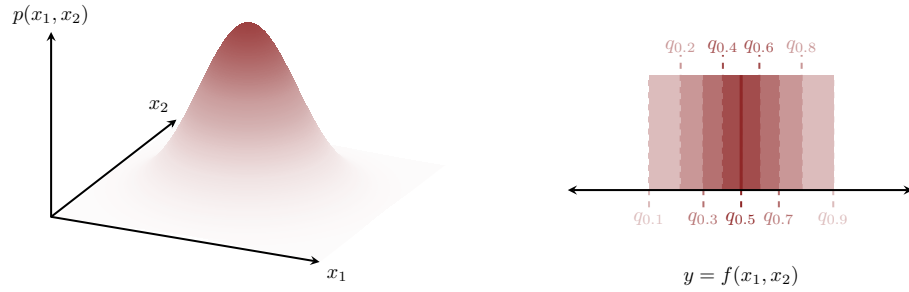

Figure 21: Nested quantile intervals provide a compact characterization of one-dimensional pushforward distributions.

is sufficiently small.

I personally find histogram characterizations to be the most robust compromise between practical feasibility and visual information density, and we will be using them often in this book. Because they can be condensed into a single line nested quantile intervals can also be convenient when visualizing many pushforward distributions at the same time (Figure 22). These visualizations are also know as **fan plots** or **ribbon plots**.

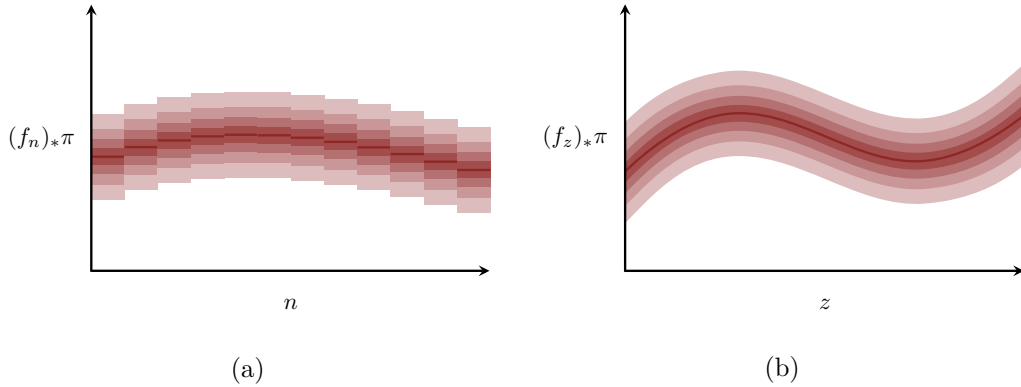(a)   (b)

Figure 22: Nested quantile intervals are particularly useful for visualizing both (a) finite collections of summary functions that can be indexed by integers $n \in \mathbb{Z}$ and (b) uncountably infinite collections of summary functions that can be indexed by real numbers $z \in \mathbb{R}$. These visualizations are somewhat limited because they don't convey the correlations between the summary function outputs but with that caveat in mind they can be incredibly effective.

6 Conclusion

The ability to transform probabilistic objects, in particular the ability to actually implement these transformations in practice, is an extremely powerful tool in applied probability theory. These transformations allow us to not only manipulate probability spaces into more convenient forms but also distill high-dimensional probabilistic information to low-dimensional summary spaces that are straightforward to visualize.

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