More categorical variables and Monte Carlo CPSC 440/550: Advanced Machine Learning

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2023-24 Winter Term 2 (Jan-Apr 2024)

Outline



- 2 Categorical MLE, MAP
- 3 Multi-class classification

Motivation: probabilistic inference

• Given a general model, we often want to make inferences

- Marginals: what's the probability that $X_i = c$?
- Conditionals: what's the probability that $X_i = c$, given that $X_{i'} = c'$?
- This has been simple for the models we've seen so far
 - For Bernoulli/categorical, computing probabilities is straightforward
 - For product of Bernoullis (or categoricals), assumed everything is independent
- For many models, inference has no closed form or might be NP-hard
- In these cases, we'll often use Monte Carlo approximations

Monte Carlo: marginalization by sampling

- A basic Monte Carlo method for estimating probabilities of events:
- Step 1: Generate a lot of samples $x^{(i)}$ from our model

$$X = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

• Step 2: Count how often the event occurred in the samples

$$\Pr(X_2 = 1) \approx \frac{3}{4} \qquad \Pr(X_3 = 0) \approx 0$$

- This very simple idea is one of the most important algorithms in ML/statistics
- Modern versions developed to build better nuclear weapons :/
 - "Sample" from a physics simulator, see how often it leads to a chain reaction

Monte Carlo to approximate probabilities

• Monte Carlo estimate of the probability of an event A:

 $\frac{\text{number of samples where } A \text{ happened}}{\text{number of samples}} = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(A \text{ happened in } x^{(i)})$

- $\bullet\,$ You can think of this as the MLE of a binary variable $\mathbbm{1}(A \text{ happened})$
- Approximating probability of a pair of independent dice adding to 7:
 - Roll two dice, check if they add to 7
 - Roll two dice, check if they add to 7
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 - Roll two dice, check if they add to 7
 - . . .
 - Monte Carlo estimate: fraction where they add to 7

Monte Carlo to approximate probabilities

- Recall the problem of modeling (Lib, CPC, NDP, GRN, PPC)
- From 100 samples, what's the probability that $n_{Lib} > \max(n_{CPC}, n_{NDP}, \dots)$?
- Can answer this in closed form with math ... or think less and do Monte Carlo
 - Generate 100 samples, check who won
 - Generate 100 samples, check who won
 - ...
 - Approximate probability by fraction of times they won
- Another example: probability that $Beta(\alpha,\beta)$ is above 0.7

Monte Carlo to estimate the mean

• A Monte Carlo estimate for the mean: the mean of the samples

$$\mathbb{E}[X] \approx \frac{1}{n} \sum_{i=1}^{n} x^{(i)}$$

• A Monte Carlo approximation of the expected value of X^2 :

$$\mathbb{E}[X^2] \approx \frac{1}{n} \sum_{i=1}^n \left(x^{(i)} \right)^2$$

• A Monte Carlo approximation of the expected value of g(X):

$$\mathbb{E}[g(X)] \approx \frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right) \qquad \mathbb{E}[g(X)] = \sum_{x \in \mathcal{X}} p(x)g(x) \text{ or } \int_{x \in \mathcal{X}} p(x)g(x) \mathrm{d}x$$

• Most general form: g(x) = x, $g(x) = x^2$, $g(x) = \mathbb{1}(A \text{ happens on } x)$

$$\mathbb{E}[\mathbbm{1}(A \text{ happens on } x)] = \int_{x \in \mathcal{X}} p(x) \,\mathbbm{1}(A \text{ happens on } x) \mathrm{d}x = \int_{x:A \text{ happens}} p(x) \mathrm{d}x = \Pr(A)$$

Monte Carlo: theory

- Let $\mu = \mathbb{E}[g(X)]$ be the value we want to compute, $\hat{\mu}$ our estimate
- Assume $\sigma^2 = \operatorname{Var}[g(X)]$ exists and is bounded ("not infinite")
- $\bullet\,$ With iid samples, Monte Carlo gives an unbiased estimate of $\mu\,$
 - Expected value of $\hat{\mu}$, over samples we might draw, is exactly μ
- \bullet Monte Carlo estimate "converges to μ " as $n \to \infty$
 - Estimate gets arbitrarily close to μ as n increases: (strong) law of large numbers
- Expected squared error is exactly $\mathbb{E}(\hat{\mu}-\mu)^2=\frac{\sigma^2}{n}$
- $\hat{\mu}$ is approximately normal with mean μ and variance $\frac{\sigma^2}{n}$ (central limit theorem)

Example application: Snakes and Ladders

bonus!

- Kid's game "Snakes and Ladders":
 - Start at 1, roll die, move the marker, follow snake/ladder
 - Absolutely no decision-making: can simulate the game
- How long does this game go for?
 - Run the game lots of times, see how many turns it took



https://www.datagenetics.com/blog/november12011/



Conditional probabilities with Monte Carlo

- "How much loooonger will this game go?"
 - Just simulate starting from current game state
- $\bullet\,$ "What's the probability the game will go $>\!100$ turns, if it's already gone 50?"
- One approach:

$$\Pr(A \mid B) = \frac{\Pr(A \cap B)}{\Pr(B)} \approx \frac{\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(A \text{ and } B \text{ happened on } x^{(i)})}{\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(B \text{ happened on } x^{(i)})}$$

- This is one instance of rejection sampling (more later)
- If B is rare, most samples are wasted

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MLE for categorical distribution

• How do we learn a categorical model?

$$\mathbf{X} = \begin{bmatrix} \mathsf{NDP} \\ \mathsf{Lib} \\ \mathsf{Lib} \\ \mathsf{CPC} \\ \vdots \end{bmatrix} \xrightarrow{\text{density estimator}} \boldsymbol{\theta} = \begin{bmatrix} \Pr(X = \mathsf{Lib}) = 0.404 \\ \Pr(X = \mathsf{NDP}) = 0.307 \\ \Pr(X = \mathsf{CPC}) = 0.216 \\ \Pr(X = \mathsf{Grn}) = 0.039 \\ \Pr(X = \mathsf{PPC}) = 0.032 \end{bmatrix}$$

• Like before, start with maximum likelihood estimation (MLE):

$$\hat{\boldsymbol{\theta}} \in \operatorname*{arg\,max}_{\boldsymbol{\theta}} p(\mathbf{X} \mid \boldsymbol{\theta})$$

- Like before, MLE will be $\theta_c = \frac{n_c}{n}$ (the portion of *c*s in the data)
- Like before, derivation is more complicated than the result

Derivation of the MLE that doesn't work

• We showed last time that the likelihood is

$$p(\mathbf{X} \mid \boldsymbol{\theta}) = \theta_1^{n_1} \cdots \theta_k^{n_k}$$

• So, the log-likelihood is

$$\log p(\mathbf{X} \mid \boldsymbol{\theta}) = n_1 \log \theta_1 + \dots + n_k \log \theta_k$$

• Take the derivative for a particular θ_c :

$$\frac{\partial}{\partial \theta_c} \log p(\mathbf{X} \mid \boldsymbol{\theta}) = \frac{n_c}{\theta_c}$$

• Set the derivative to zero:

$$\frac{n_c}{\theta_c} = 0$$

• ... huh?

Fixing the derivation

- Setting the derivative to zero doesn't work
 - Ignores the constraint that $\sum_c \theta_c = 1$
- Some ways to enforce constraints (see e.g. this StackExchange thread):
 - Use "Lagrange multipliers," find stationary point of the "Lagrangian"
 - Define $\theta_k = 1 \sum_{c=1}^{k-1} \theta_c$, replace in the objective function
- We'll take a different way:
 - Use a different parameterization $\tilde{\theta}_c$ that doesn't have this constraint
 - Compute the MLE for the $\tilde{ heta}_c$ by setting derivative to zero
 - Convert from the $\tilde{\theta}_c$ to θ_c

Unnormalized parameterization

• Let's have $\tilde{\theta}_c$ be unnormalized:

$$\Pr(X = c \mid \tilde{\theta}_1, \dots, \tilde{\theta}_k) \propto \tilde{\theta}_c$$

• Still need each
$$\tilde{\theta}_c \geq 0$$

Can then find

$$p(c \mid \tilde{\boldsymbol{\theta}}) = \frac{\tilde{\theta}_c}{\sum_{i=1}^k \tilde{\theta}_c} = \frac{\tilde{\theta}_c}{Z_{\tilde{\boldsymbol{\theta}}}}$$

- The "normalizing constant" $Z_{\tilde{\theta}}$ makes the total probability 1
 - Don't need the explicit sum-to-1 constraint anymore
 - Note: constant for different x; **not** constant for different θ
- To convert from unnormalized to normalized: $\theta_c = \tilde{\theta}_c/Z_{\tilde{\theta}}$

Derivation of the MLE that does work

• The likelihood in terms of the unnormalized parameters is

$$p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}}) = \left(\frac{\tilde{\theta}_1}{Z_{\tilde{\boldsymbol{\theta}}}}\right)^{n_1} \cdots \left(\frac{\tilde{\theta}_k}{Z_{\tilde{\boldsymbol{\theta}}}}\right)^{n_k} = \frac{1}{Z_{\tilde{\boldsymbol{\theta}}}^n} \tilde{\theta}_1^{n_1} \cdots \tilde{\theta}_k^{n_k}$$

• So, the log-likelihood is

$$\log p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}}) = n_1 \log \tilde{\theta}_1 + \dots + n_k \log \tilde{\theta}_k - n \log Z_{\tilde{\boldsymbol{\theta}}}$$

• Take the derivative for a particular $\tilde{\theta}_c$:

$$\frac{\partial}{\partial \tilde{\theta}_c} \log p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}}) = \frac{n_c}{\tilde{\theta}_c} - \frac{n}{Z_{\tilde{\boldsymbol{\theta}}}} \frac{\partial Z_{\tilde{\boldsymbol{\theta}}}}{\partial \tilde{\theta}_c} = \frac{n_c}{\tilde{\theta}_c} - \frac{n}{Z_{\tilde{\boldsymbol{\theta}}}} \qquad \text{since } \frac{\partial}{\partial \tilde{\theta}_c} \left(\tilde{\theta}_1 + \dots + \tilde{\theta}_k \right) = 1$$

• Set the derivative to zero:

$$rac{n_c}{ ilde{ heta}_c} = rac{n}{Z_{ ilde{ heta}}} \quad ext{ so } \quad rac{ heta_c}{Z_{ ilde{ heta}}} = rac{n_c}{n}$$

 \sim

- Can check this objective is concave, so this is a max
- Many solutions, but all the same after normalizing

MAP estimate, Dirichlet prior

- As before, might prefer MAP estimate over MLE
- Often becomes more important for large k: lots of parameters!
- Most common prior is the Dirichlet distribution:

$$p(\theta_1,\ldots,\theta_k \mid \alpha_1,\ldots,\alpha_k) \propto \theta_1^{\alpha_1-1} \cdots \theta_k^{\alpha_k-1}$$

- $\bullet\,$ Generalization of the beta distribution to k classes
- Requires each $\alpha_c > 0$
- This is a distribution over heta
 - Probability distribution over possible (categorical) probability distributions

Dirichlet distribution

• Wikipedia's visualizations for k = 3:



https://en.wikipedia.org/wiki/Dirichlet_distribution

MAP estimate for Dirichlet-Categorical

• Reason to use the Dirichlet: again because posterior is simple

$$p(\boldsymbol{\theta} \mid \mathbf{X}, \boldsymbol{\alpha}) \propto p(\mathbf{X} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \boldsymbol{\alpha}) \propto \theta_1^{n_1} \cdots \theta_k^{n_k} \theta_1^{\alpha_1 - 1} \cdots \theta_k^{\alpha_k - 1}$$
$$= \theta_1^{(n_1 + \alpha_1) - 1} \cdots \theta_k^{(n_k + \alpha_k) - 1}$$

i.e. it's Dirichlet again with parameters $\tilde{\alpha}_c = n_c + \alpha_c$

• A few more steps show MAP for a categorical with Dirichlet prior is

$$\hat{\theta}_{c} = \frac{n_{c} + \alpha_{c} - 1}{\sum_{c'=1}^{k} (n_{c'} + \alpha_{c'} - 1)}$$

- Dirichlet has k hyper-parameters α_c
 - Often use $\alpha_c = \alpha$ for some $\alpha \in \mathbb{R}$: one hyperparameter
 - Makes the MLE $\hat{\theta}_c = \frac{n_c + \alpha 1}{n + k(\alpha 1)}$
 - $\alpha = 2$ gives Laplace smoothing (add 1 "fake" count for each class)

Conjugate priors

- This is our second example where prior and posterior have the same form
 - Beta prior + Bernoulli likelihood gives a Beta posterior
 - Also happens with binomial, geometric, ... likelihoods
 - Dirichlet prior + categorical likelihood gives a Dirichlet posterior
 - Also happens with multinomial likelihood
- When this happens, we say prior is conjugate to the likelihood
- Prior and posterior come from the same "family" of distributions

 $X \sim L(\theta) \quad \theta \sim P(\lambda) \qquad \text{implies} \quad \theta \mid X \sim P(\lambda')$

- $\bullet~$ Updated parameters λ will depend on the data
- Many computations become easier if we have a conjugate prior
- But not all distributions have conjugate priors
 - And even when one exists, might not be convenient

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Multi-class classification

• Often have classification with categorical labels and/or features

| | Cough | Low fever | Normal breathing | | [Cold] |
|----------------|----------|--------------|---------------------|----------------|-----------|
| | Cough | High fever | Shortness of breath | | Pneumonia |
| $\mathbf{X} =$ | No cough | High fever | Normal breathing | $\mathbf{y} =$ | Covid |
| | No cough | Low fever | Normal breathing | | Covid |
| | Cough | Medium fever | Normal breathing | | Cold |

- Can adapt all of our previous binary classification methods:
 - Naïve Bayes
 - Tabular probabilities
 - Logistic regression / neural nets

Product of categoricals, multi-class Naïve Bayes

- Start: multivariate categorical density estimation
 - Input: $n \ {\rm iid} \ {\rm samples} \ {\rm of} \ {\rm categorical} \ {\rm vectors} \ x^{(1)}, \ldots, x^{(n)}$
 - Output: model giving probability for any assignment of values x_1,\ldots,x_d

| $\mathbf{X} =$ | Α | С | С | Т | Т | Т | Α | G | C | $\xrightarrow{\text{density estimator}}$ | ÷ | | | |
|----------------|---|---|---|---|---|---|---|---|---|--|---|--|--|--|
| | Α | С | С | G | Т | Т | Α | G | G | | | | | |
| | Α | С | С | Т | Т | Т | А | G | С | | $\Pr(X_1 = \mathbf{A}, X_2 = \mathbf{C}, \dots, X_9 = \mathbf{C}) = 0.11$ | | | |
| | Α | А | С | Т | Т | Т | С | G | G | | $(4^9$ possible values) | | | |

• Like for product of Bernoullis, we could use product of categoricals

• Assumes X_j are mutually independent: strong assumption that makes things easy

$$\Pr(X_1 = c_1, \dots, X_d = c_d) = \Pr(X_1 = c_1) \dots \Pr(X_d = c_d) = \theta_{1,c} \cdots \theta_{d,c_d}$$

- Parameter $\theta_{j,c}$ is probability that jth entry is in cth class
- \bullet Like before, could use product of categoricals conditional on Y to get categorical naïve Bayes

Multi-class naïve Bayes on MNIST

- Binarized MNIST: label is categorical, but images are still product of Bernoullis
- Parameter of the Bernoulli for each class:



• One sample from each class:



Tabular probabilities for categorical data

• Can use a tabular parameterization: with two binary features, three-way label,

$$\begin{aligned} &\Pr(Y=1 \mid X_1=0, X_2=0) = \theta_{1\mid 00} & \Pr(Y=2 \mid X_1=0, X_2=0) = \theta_{2\mid 00} & \Pr(Y=3 \mid X_1=0, X_2=0) = \theta_{3\mid 00} \\ &\Pr(Y=1 \mid X_1=0, X_2=1) = \theta_{1\mid 01} & \Pr(Y=2 \mid X_1=0, X_2=1) = \theta_{2\mid 01} & \Pr(Y=3 \mid X_1=0, X_2=1) = \theta_{3\mid 01} \\ &\Pr(Y=1 \mid X_1=1, X_2=0) = \theta_{1\mid 10} & \Pr(Y=2 \mid X_1=1, X_2=0) = \theta_{2\mid 10} & \Pr(Y=3 \mid X_1=1, X_2=0) = \theta_{3\mid 10} \\ &\Pr(Y=1 \mid X_1=1, X_2=1) = \theta_{1\mid 11} & \Pr(Y=2 \mid X_1=1, X_2=1) = \theta_{2\mid 11} & \Pr(Y=3 \mid X_1=1, X_2=1) = \theta_{3\mid 11} \end{aligned}$$

- Don't necessarily need $\theta_{3|x};$ can use $\theta_{3|x}=1-\theta_{1|x}-\theta_{2|x}$
- MLE has simple closed form: $\hat{ heta}_{y|x} = n_{y|x}/n_x$
 - Just the categorical MLE for each condition
- Can use a Dirichlet (or whatever other) prior and do MAP
- Will overfit unless you have small number of distinct x

Parameterizing conditionals

- Tabular treats each $\theta_{y|x}$ totally separately
- \bullet Could instead share information for "similar" x
 - Can no longer express every possible distribution, potentially computationally harder
 - Statistically much easier to fit
- One choice: weight w_c for each class, get $z_c = w_c^{\mathsf{T}} x$ for each c
- Need to turn the z_c into parameters of a categorical distribution
- Binary data: mapped one z into (0,1) with sigmoid $f(z)=1/(1+\exp(-z))$ • But using $\theta_c=f(z_c)$ won't sum to one
- \bullet Softmax function first makes nonnegative by taking $\exp,$ then normalizes:

$$\theta_c = [\operatorname{softmax}(\mathbf{z})]_c = \frac{\exp(z_c)}{\sum_{c'=1}^k \exp(z_{c'})} \propto \exp(z_c)$$

• Don't have to use softmax, other options exist, but this is default

Categorical features as inputs

- How do we use categorical data in the features x?
- Usually convert to set of binary features ("one-hot" / "one of k" encoding)

| Age | City | Income | | Age | Van | Bur | Sur | Income |
|-----|------|---------|---------------|-----|-----|-----|-----|---------|
| 23 | Van | 26,000 | | 23 | 1 | 0 | 0 | 26,000 |
| 25 | Sur | 67,000 | \rightarrow | 25 | 0 | 0 | 1 | 67,000 |
| 19 | Bur | 16,500 | | 19 | 0 | 1 | 0 | 16,500 |
| 43 | Sur | 183,000 | | 43 | 0 | 0 | 1 | 183,000 |

• If you see a new category in test data: usually, just set all of them to zero

Softmax and binary logistic regression

• With two categories: using a "dummy" value $z_2 = 0$

$$[\operatorname{softmax}((z,0))]_1 = \frac{\exp(z)}{\exp(z) + \exp(0)} \times \frac{\exp(-z)}{\exp(-z)} = \frac{1}{1 + \exp(-z)}$$

• Two-class softmax regression with one weight frozen at zero is logistic regression



Softmax loss

• Taking the negative log-likelihood:

$$-\log p(\mathbf{y} \mid W, \mathbf{X}) = -\sum_{i=1}^{n} \log p(y^{(i)} \mid W, x^{(i)}) = -\sum_{i=1}^{n} \left[\log \left(\frac{\exp \left(w_{y^{(i)}}^{\mathsf{T}} x^{(i)} \right)}{\sum_{c=1}^{k} \exp(w_{c}^{\mathsf{T}} x^{(i)})} \right) \right]$$
$$= \sum_{i=1}^{n} \left[-w_{y^{(i)}}^{\mathsf{T}} x^{(i)} + \log \left(\sum_{c=1}^{k} \exp(w_{c}^{\mathsf{T}} x^{(i)}) \right) \right]$$

- Convex (note log-sum-exp is convex), differentiable: can use gradient descent
- Often add a regularizer (i.e. a prior on W)
- Gradient has a nice form:

$$\frac{\partial}{\partial w_c} [-\log p(\mathbf{y} \mid W, \mathbf{X})] = -\sum_{i=1}^n \mathbb{1}(y^{(i)} = c)x^{(i)} + \sum_{i=1}^n \underbrace{\frac{\exp(w_c^\mathsf{T} x^{(i)})}{\sum_{c'=1}^k \exp(w_c^\mathsf{T} x^{(i)})}}_{p(y^{(i)} = c|x^{(i)}, W)} x^{(i)}$$

Multi-label versus multi-class classification

- Before: we saw multi-label classification, where y is a binary vector of length k • "This image has a chair and a person, but no frog"
- Multi-class, e.g. with softmax loss: y has exactly one of k discrete labels
 "This is an image of a frog"
- Could have multiple categorical labels (some of which might be binary)
 "This paper's arXiv primary class is stat.ML, and the first author is a student"



Monte Carlo is a general way to estimate expectations when you can sample
 Including probabilities: expectations of indicators

• Next time: everything is regularization

Law of the Unconscious Statistician



• These inequalities sometimes called "Law of the Unconscious Statistician":

$$\mathbb{E}[g(X)] = \sum_{x \in \mathcal{X}} g(x)p(x) \qquad \mathbb{E}[g(X)] = \int_{x \in \mathcal{X}} g(x)p(x)dx$$

- Two explanations I've heard for "unconscious":
 - You can compute expectations without thinking
 - Or: people don't realize this is actually a theorem to prove, not a definition

$$\mathbb{E}[Y] = \sum_{y} y \operatorname{Pr}(Y = y) = \sum_{y} y \sum_{x:g(x)=y} p(x) = \sum_{x} g(x)p(x)$$

bonus!

Mean and Variance of Monte Carlo

•
$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} g(x^{(i)})$$
 is an unbiased estimate of $\mu = \mathbb{E}[g(x)]$:

$$\mathbb{E}\left[\frac{1}{n} \sum_{i=1}^{n} g(x^{(i)})\right] = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}\left[g(x^{(i)})\right] = \frac{1}{n} \sum_{i=1}^{n} \mu = \mu$$

• If $\operatorname{Var}(g(x^{(i)})) = \sigma^2$ for some finite σ , then

$$\operatorname{Var}\left(\frac{1}{n}\sum_{i=1}^{n}g(x^{(i)})\right) = \frac{1}{n^2}\sum_{i=1}^{n}\underbrace{\operatorname{Var}\left(g(x^{(i)})\right)}_{\sigma^2} - \frac{2}{n^2}\sum_{i\neq j}\underbrace{\operatorname{Cov}\left(g(x^{(i)}), g(x^{(j)})\right)}_{0} = \frac{1}{n^2}n\sigma^2 = \frac{\sigma^2}{n}$$

• Expected squared error is σ^2/n :

$$\mathbb{E}\left[\left(\frac{1}{n}\sum_{i=1}^{n}g(x^{(i)})-\mu\right)^{2}\right] = \left(\mathbb{E}\frac{1}{n}\sum_{i=1}^{n}g(x^{(i)})-\mu\right)^{2} + \operatorname{Var}\left(\frac{1}{n}\sum_{i=1}^{n}g(x^{(i)})\right) = 0 + \frac{\sigma^{2}}{n}$$

Monte Carlo as a stochastic gradient method



Can view as SGD on $f(\hat{\mu}) = \frac{1}{n} ||\hat{\mu} - \mu||^2$ with learning rate $\frac{1}{i+1}$:

$$\dot{\mu}_{n} = \hat{\mu}_{n-1} - \frac{1}{n} \left(\hat{\mu}_{n-1} - x^{(i)} \right)$$

$$= \left(1 - \frac{1}{n} \right) \hat{\mu}_{n-1} + \frac{1}{n} x^{(i)}$$

$$= \frac{n-1}{n} \left(\frac{1}{n-1} \sum_{i=1}^{n-1} x^{(i)} \right) + \frac{1}{n} x^{(i)}$$

$$= \frac{1}{n} \sum_{i=1}^{n-1} x^{(i)} + \frac{1}{n} x^{(i)} = \frac{1}{n} \sum_{i=1}^{n} x^{(i)}$$