Optimal Stein-type Goodness-of-Fit Tests for Count Data

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Using Stein Identities for Goodness-of-Fit Tests

Introduction

Using Stein Identities for GoF-Tests

Idea to characterize given distribution family by appropriate moment identity dates back to Stein (1972). **Stein identities** also available for several count distributions, see Sudheesh & Tibiletti (2012), Betsch et al. (2022), Weiß & Aleksandrov (2022). Among others,

- $X \sim \text{Poi}(\mu)$ iff $\quad E\big[X\, f(X)\big] \;=\; \mu\, E\big[f(X+1)\big]$
  holds for all bounded functions $f: \mathbb{N}_0 \to \mathbb{R}$;
- $X \sim \text{Bin}(N, \pi)$ with mean $\mu = N\,\pi$ iff

$$(N-\mu)\, E\big[X\, f(X)\big] \;=\; \mu\, E\big[(N-X)\, f(X+1)\big]$$

holds for all bounded functions $f: \mathbb{N}_0 \to \mathbb{R}$.

Using Stein Identities for GoF-Tests

Recently, Stein identities utilized to define GoF-tests, e. g., by Aleksandrov et al. (2022a,b) and Betsch et al. (2022).

Here, we follow idea of Aleksandrov et al. (2022a,b) and consider moment-based GoF-statistics, such as

$$\hat{\mathsf{T}}_{f;\,\mathsf{Poi}} = \frac{\overline{X\,f(X)}}{\overline{X}\ \overline{f(X+1)}} \quad \text{and} \quad \hat{\mathsf{T}}_{f;\,\mathsf{Bin}} = \frac{\left(N-\overline{X}\right)\ \overline{X\,f(X)}}{\overline{X}\ \overline{(N-X)\,f(X+1)}},$$

where $\overline{\boldsymbol{g}(X)} = \frac{1}{n}\sum_{t=1}^{n}\boldsymbol{g}(X_t)$.

Deviations from 1 indicate violation of Poi-/Bin-assumption.

Idea: weight function f selected by user from given class $\mathcal{F}$ to ensure good power properties for specified alternative.

Examples for the choice of $\mathcal{F}$:

- Power weighting scheme $f_a(x) = |x-1|^a$ with $a > 0$,

$$\hat{\mathsf{T}}_{f_a;\,\mathsf{Poi}} = \frac{\overline{X\,(X-1)^a}}{\overline{X}\;\overline{X^a}}$$

  where $a = 1$ corresponds to dispersion index (“U-test”).

  $a < 1$ leads to root weights, for example, while

  $a = 2$ leads to kind of skewness statistic.

- Exponential-type functions $f_u(x) = u^x$ with $u \in (0;1)$,

  motivated by probability generating function.

- Functions $f_d(x) = (x+1)^{-d}$ with $d > 0$

  put most weight on low counts.

Advantages of moment-based GoF-statistics:

We can derive closed-form asymptotics

both under null and specified alternative. Hence,

1. asymptotic critical values such that GoF-test easily implemented in practice (no need for bootstrap),
2. determine optimal $f \in \mathcal{F}$ for considered alternative by maximizing asymptotic power.

In what follows, approach demonstrated and investigated for Poisson or binomial counts, but easily adapted to other distributions (e. g., negative-binomial in Weiß et al. (2023)).

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Stein-type Poi-GoF test: Asymptotic Power Analysis

Derivation & Application

Notation: For given $f \in \mathcal{F}$, $k \geq 0$, and $0 \leq l_1 \leq \ldots \leq l_m$, let

$$\mu(k; l_1, \ldots, l_m) \ := \ E\big[X^k \cdot f(X + l_1) \cdots f(X + l_m)\big].$$

Reduces to $\mu(k) = E\big[X^k\big]$ if $m = 0$. These moments computed either exactly, or numerically approximated by

$$\mu(k; l_1, \ldots, l_m) \ \approx \ \sum_{x=0}^{M} x^k \cdot f(x + l_1) \cdots f(x + l_m) \cdot P(X = x).$$

Example: Population counterpart to $\hat{\mathsf{T}}_{f;\,\mathsf{Poi}}$ computes as

$$\mathsf{T}_{f;\,\mathsf{Poi}} \ := \ \frac{E\big[X\, f(X)\big]}{E[X]\, E\big[f(X+1)\big]} \ = \ \frac{\mu(1; 0)}{\mu\, \mu(0; 1)}.$$

Under H_0: $X \sim \mathsf{Poi}(\mu)$, it holds $\quad \mathsf{T}_{f;\,\mathsf{Poi}} = 1.$

Stein Poi-GoF test: Asymptotic Power Analysis

Theorem 1: For i. i. d. $X_1, \ldots, X_n$, $\hat{\mathsf{T}}_{f;\,\mathsf{Poi}}$ approximately normal, $\mathsf{N}\big(\mu_{f;\,\mathsf{Poi}},\ \sigma^2_{f;\,\mathsf{Poi}}/n\big)$, where bias-corrected mean

$$\mu_{f;\,\mathsf{Poi}} = \mathsf{T}_{f;\,\mathsf{Poi}} + \frac{1}{n}\mathsf{T}_{f;\,\mathsf{Poi}}\left(\frac{\sigma_{11}}{\mu^2} + \frac{\sigma_{33}}{\mu(0;1)^2} - \frac{\sigma_{12}}{\mu\,\mu(1;0)} + \frac{\sigma_{13}}{\mu\,\mu(0;1)} - \frac{\sigma_{23}}{\mu(1;0)\,\mu(0;1)}\right),$$

and asymptotic variance

$$\sigma^2_{f;\,\mathsf{Poi}} = \mathsf{T}^2_{f;\,\mathsf{Poi}}\left(\frac{\sigma_{11}}{\mu^2} + \frac{\sigma_{22}}{\mu(1;0)^2} + \frac{\sigma_{33}}{\mu(0;1)^2} - \frac{2\,\sigma_{12}}{\mu\,\mu(1;0)} + \frac{2\,\sigma_{13}}{\mu\,\mu(0;1)} - \frac{2\,\sigma_{23}}{\mu(1;0)\,\mu(0;1)}\right).$$

Here, the required expressions for σ_{ij} are

$$\begin{aligned}
\sigma_{11} &= \sigma^2, & \sigma_{12} &= \mu(2;0) - \mu\,\mu(1;0),\\
\sigma_{13} &= \mu(1;1) - \mu\,\mu(0;1), & \sigma_{22} &= \mu(2;0,0) - \mu(1;0)^2,\\
\sigma_{23} &= \mu(1;0,1) - \mu(1;0)\,\mu(0;1), & \sigma_{33} &= \mu(0;1,1) - \mu(0;1)^2.
\end{aligned}$$

Theorem 1 used to test Poisson null hypothesis.

1. Compute asymptotics by plugging-in Poi(μ)-pmf $\Rightarrow$ **critical values** of (two-sided) $\hat{\mathsf{T}}_{f;\,\mathsf{Poi}}$-test on level α:

   $$\text{reject Poi-null iff} \quad \hat{\mathsf{T}}_{f;\,\mathsf{Poi}} \notin \Big[\mu_0 - z_{1-\frac{\alpha}{2}}\,\sigma_0\ ;\ \mu_0 + z_{1-\frac{\alpha}{2}}\,\sigma_0\Big].$$

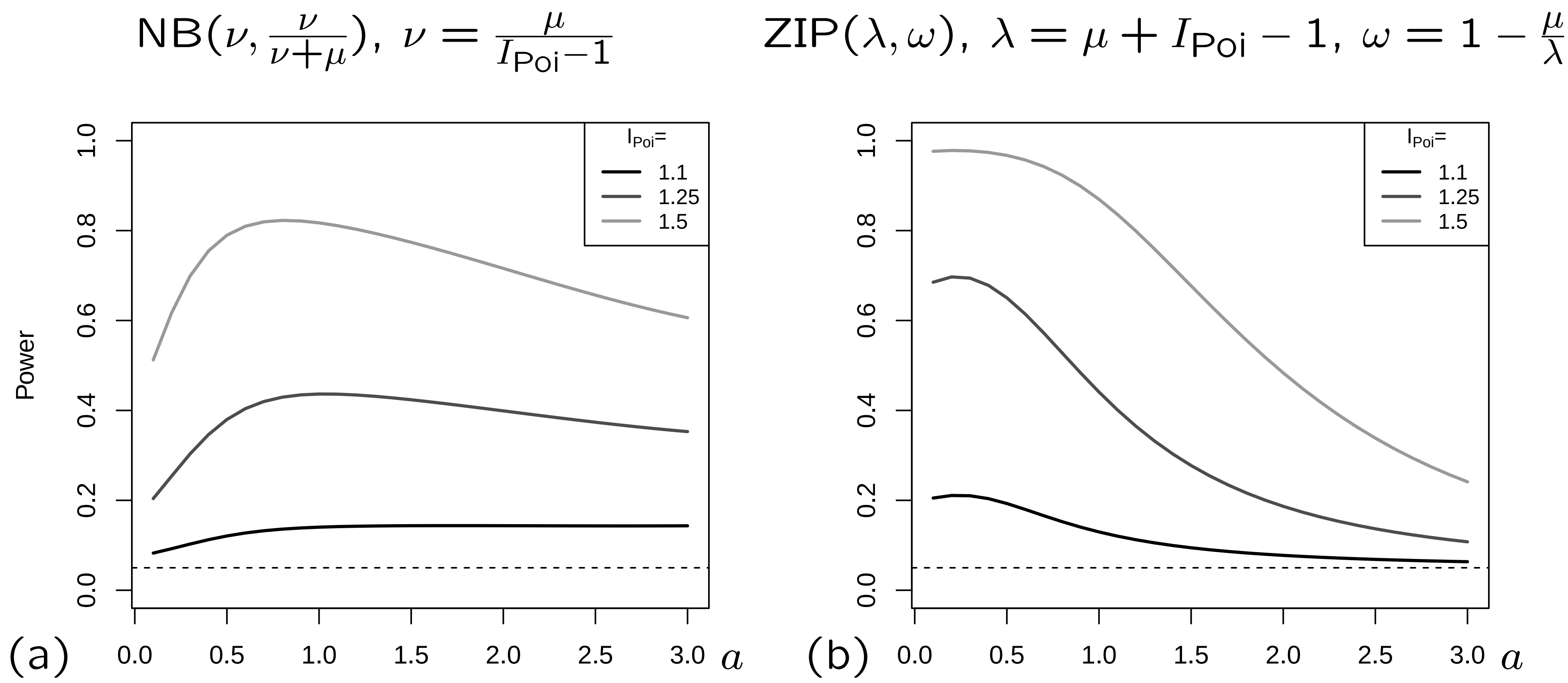
2. Compute **asymptotic power** for given alternative by plugging-in alternative's pmf into Theorem 1.

   f optimal within $\mathcal{F}$ if f maximizes asymptotic power, i. e., we select

   $$\arg\max_{f\in\mathcal{F}}\ P\Big(\big|\hat{\mathsf{T}}_{f;\,\mathsf{Poi}} - \mu_0\big| > z_{1-\frac{\alpha}{2}}\,\sigma_0\Big).$$

Examples: Asymptotic power for Poi(2)-null ($n = 100$) against overdispersed NB- or ZIP-alternative ($I_{\text{Poi}} = \frac{\sigma^2}{\mu} > 1$).

$\mathcal{F} = \{|x-1|^a \mid a \in (0;3)\}$

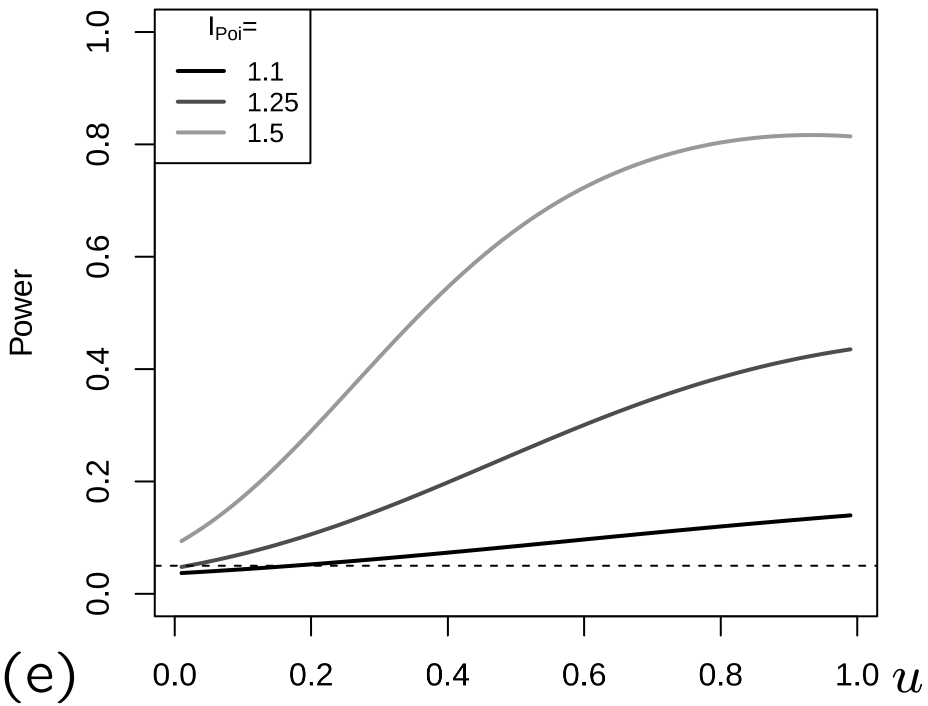


Stein Poi-GoF test: Asymptotic Power Analysis

Examples: Asymptotic power for Poi(2)-null ($n = 100$) against overdispersed NB- or ZIP-alternative ($I_{\text{Poi}} = \frac{\sigma^2}{\mu} > 1$).

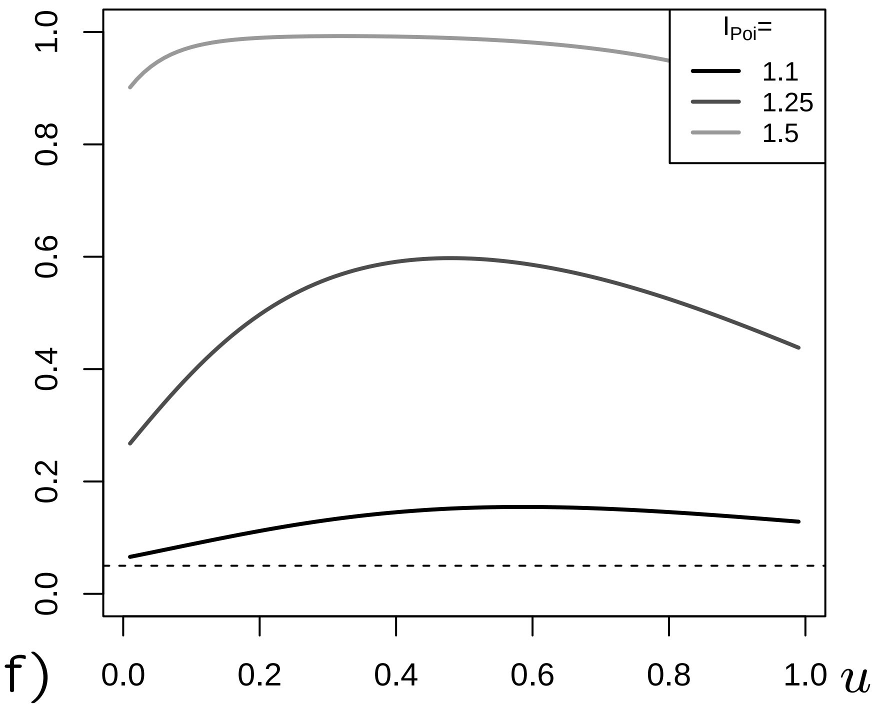
$\mathcal{F} = \{u^x \mid u \in (0;1)\}$

$\text{NB}(\nu, \frac{\nu}{\nu+\mu})$, $\nu = \frac{\mu}{I_{\text{Poi}}-1}$



(e)

$\text{ZIP}(\lambda, \omega)$, $\lambda = \mu + I_{\text{Poi}} - 1$, $\omega = 1 - \frac{\mu}{\lambda}$

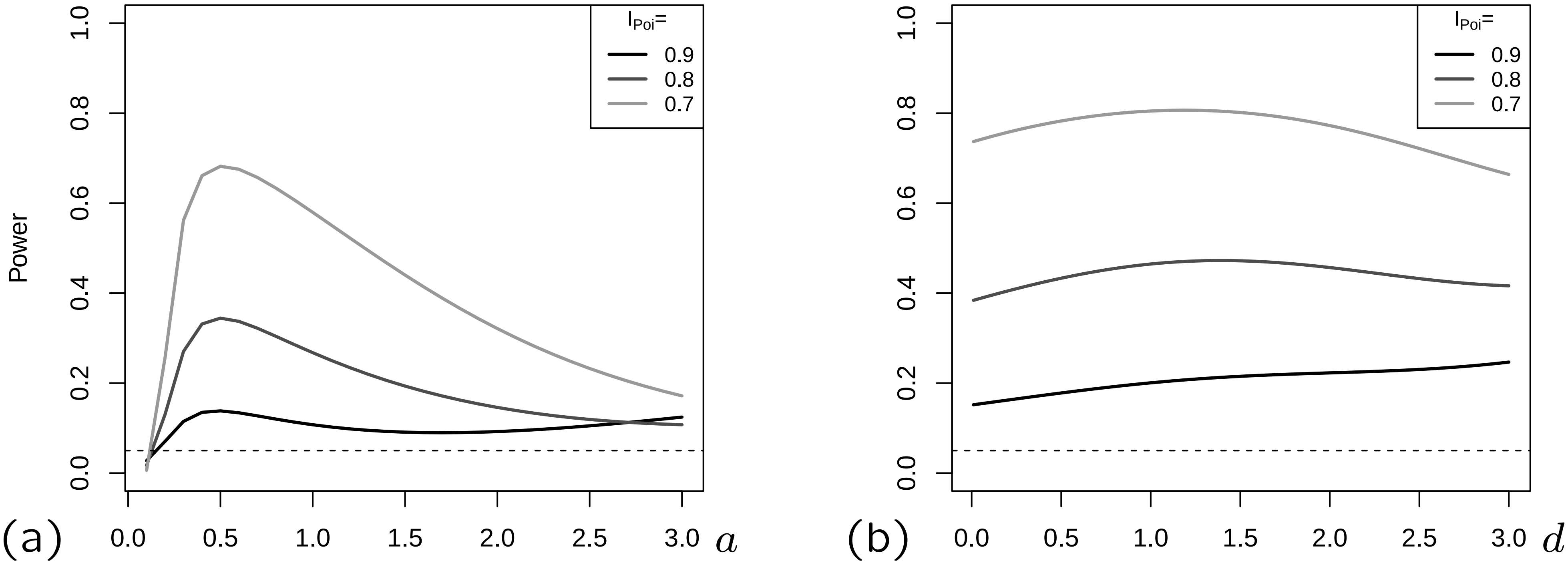


(f)

Examples: Asymptotic power for Poi(4)-null ($n = 100$) against underdispersed Good alternative ($I_{\text{Poi}} = \frac{\sigma^2}{\mu} < 1$).

Good(β, δ)

$\mathcal{F} = \{|x-1|^a \mid a \in (0;3)\}$ $\mathcal{F} = \{(x+1)^{-d} \mid d \in (0;3)\}$



(a) (b)

Theorem 2: For i. i. d. $X_1,\ldots,X_n$, $\hat{\mathsf{T}}_{f;\,\mathsf{Bin}}$ approximately normal, $\mathsf{N}\big(\mu_{f;\,\mathsf{Bin}},\ \sigma^2_{f;\,\mathsf{Bin}}/n\big)$, where bias-corrected mean

$$\mu_{f;\,\mathsf{Bin}} = \mathsf{T}_{f;\,\mathsf{Bin}} + \frac{1}{n}\mathsf{T}_{f;\,\mathsf{Bin}}\Bigg(\frac{N}{N-\mu}\,\frac{\sigma_{11}}{\mu^2} + \frac{\sigma_{33}}{\big(N\mu(0;1)-\mu(1;1)\big)^2} - \frac{N}{N-\mu}\,\frac{\sigma_{12}}{\mu\,\mu(1;0)} + \frac{N}{N-\mu}\,\frac{\sigma_{13}}{\mu\,\big(N\mu(0;1)-\mu(1;1)\big)} - \frac{\sigma_{23}}{\mu(1;0)\,\big(N\mu(0;1)-\mu(1;1)\big)}\Bigg),$$

and asymptotic variance

$$\sigma^2_{f;\,\mathsf{Bin}} = \mathsf{T}^2_{f;\,\mathsf{Bin}}\Bigg(\frac{N^2}{(N-\mu)^2}\,\frac{\sigma_{11}}{\mu^2} + \frac{\sigma_{22}}{\mu(1;0)^2} + \frac{\sigma_{33}}{\big(N\mu(0;1)-\mu(1;1)\big)^2} - \frac{2\,N}{N-\mu}\,\frac{\sigma_{12}}{\mu\,\mu(1;0)} + \frac{2\,N}{N-\mu}\,\frac{\sigma_{13}}{\mu\,\big(N\mu(0;1)-\mu(1;1)\big)} - \frac{2\,\sigma_{23}}{\mu(1;0)\,\big(N\mu(0;1)-\mu(1;1)\big)}\Bigg).$$

Here, the required expressions for σ_{ij} are . . .

see Weiß et al. (2023).

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Real-World Data Examples

Illustration

Data Application: Biological Dosimetry

Pujol et al. (2016) conducted experiment where blood samples from two donors, male and female, irradiated at different doses. Samples mixed in 1:1 ratio to construct heterogeneous exposures. Data sets from their Table 1B, where, e. g., "M4F1" indicates that male received 4 Gy of radiation and female 1 Gy.

Observed dicentric distributions confronted with Poisson null. Conjectured alternative scenario:
$X \sim \text{MixPoi}(\lambda_1, \lambda_2, \omega)$ with $\lambda_1, \lambda_2 > 0$ and $\omega \in (0;1)$ iff

$$P(X = x) \;=\; \omega\, e^{-\lambda_1} \frac{\lambda_1^x}{x!} \;+\; (1-\omega)\, e^{-\lambda_2} \frac{\lambda_2^x}{x!} \qquad \text{for } x \in \mathbb{N}_0.$$

Here, $\omega = 0.5$ because 1:1 ratio for blood mixtures.

Optimal $\hat{T}_{f;\,\text{Poi}}$-tests with $f(x) = |x-1|^a$, MixPoi-alternative.

n_i	$\hat{\mu}_i$	I_{Poi}	a_{opt}	asym. power	$\hat{T}_{f;\,\text{Poi}}$	critical values lower	critical values upper	U-test power	KS-test power	LR-test power
399	0.501	1.10	0.951	0.319	1.946	0.722	1.268	0.305	0.086	0.367
("M4F1")		1.25	0.571	0.900	2.031	0.742	1.253	0.881	0.360	0.926
		1.50	0.319	1.000	2.088	0.745	1.253	1.000	0.970	1.000
326	0.629	1.10	0.988	0.277	1.940	0.752	1.238	0.267	0.099	0.323
("F4M1")		1.25	0.644	0.844	1.948	0.774	1.221	0.822	0.368	0.878
		1.50	0.387	1.000	1.948	0.780	1.217	1.000	0.948	1.000
288	0.698	1.10	1.006	0.255	1.741	0.760	1.230	0.243	0.087	0.295
("M6F2")		1.25	0.676	0.803	1.665	0.783	1.210	0.779	0.326	0.843
		1.50	0.424	0.999	1.595	0.791	1.205	0.999	0.913	1.000
264	0.758	1.10	1.018	0.240	2.168	0.768	1.222	0.230	0.086	0.279
("F6M2")		1.25	0.700	0.773	2.091	0.792	1.202	0.745	0.305	0.813
		1.50	0.454	0.998	2.013	0.800	1.196	0.998	0.886	0.999

$I_{\text{Poi}} = \sigma^2/\mu$

Data Application: Dental Health

Dental health of children, see Böhning et al. (1999).

DMFT counts (“decayed, missing and filled teeth”)

on deciduous molars, so upper bound $N = 8$.

For DMFT data (binomial null), ZIB alternative most relevant as zeros represent caries-free children.

These consist of two subgroups, see Mwalili et al. (2008):

- children that cannot have decayed teeth because of, e. g., genetic reasons, and
- children having no caries despite generally being prone to caries development.

ZIB parameter $\omega \approx$ proportion of caries-resistant children.

Optimal $\hat{T}_{f;\,\mathrm{Bin}}$-tests with $f(x) = |x-1|^a$ or $f(x) = u^x$.

n_i	$\widehat{\mu}_i$	I_{Bin}	a_{opt}	asym. power	$\hat{T}_{f;\,\mathrm{Bin}}$	u^x power	U-test power	0-index power	KS-test power	LR-test power
124	1.863	1.10	0.242	0.251	1.279	0.177	0.150	0.217	0.076	0.283
(School 1)		1.25	0.232	0.784	1.277	0.696	0.538	0.759	0.281	0.820
		1.50	0.215	0.992	1.275	0.999	0.965	0.998	0.868	0.999
127	1.307	1.10	0.294	0.210	1.768	0.161	0.148	0.177	0.089	0.244
(School 2)		1.25	0.280	0.728	1.762	0.643	0.541	0.684	0.321	0.763
		1.50	0.258	0.990	1.753	0.997	0.970	0.996	0.865	0.998
136	2.346	1.10	0.198	0.324	1.321	0.218	0.163	0.285	0.059	0.348
(School 3)		1.25	0.190	0.856	1.319	0.795	0.570	0.853	0.233	0.889
		1.50	0.177	0.996	1.315	1.000	0.970	0.999	0.865	1.000
132	2.152	1.10	0.215	0.293	1.378	0.201	0.158	0.256	0.062	0.321
(School 4)		1.25	0.206	0.832	1.376	0.759	0.560	0.820	0.220	0.865
		1.50	0.192	0.995	1.372	1.000	0.971	0.999	0.838	1.000

$I_{\mathrm{Bin}} = N\sigma^2/\mu/(N-\mu)$

Conclusions

- Stein GoF-test have moment-based statistic and closed-form asymptotics. We established Poi- and Bin-GoF test, but easily adapted to other null models.
- Asymptotics used to find optimal weighting function regarding considered specified alternative.
- Asymptotics of Theorems 1 and 2 are universally applicable: without any novel derivations, Stein GoF-test optimized for given alternative scenario.
- Clearly outperform most competitors, can be tuned to have power close to more sophisticated LR-test.

Thank You for Your Interest!

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