A Gentle Introduction to Stein’s Method for Normal Approximation III

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III. Exchangeable Pair, Zero Bias Couplings

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III. Stein Exchangeable Pair

(a) Linearity Condition
(b) Mean, Variance, Function Identities
(c) Smooth function bound

III. Zero Bias Couplings

(a) Fixed point zero bias rationale for CLT
(b) Change 1 property
(c) $L^1$ bound
(d) Connection to the Stein pair, $K$ function
Stein Equation

Let \( W \) satisfy \( EW = 0, \) \( \text{Var}(W) = 1. \) Recall, for given \( h \in \mathcal{H}, \)

\[
f'(w) - wf(w) = h(w) - Nh \quad \text{where} \quad Nh = Eh(Z).
\]

For the given \( W, \) we calculate

\[
Eh(W) - Nh
\]

by computing

\[
E[f'(W) - Wf(W)].
\]
We say the random variables \((W, W')\) form a \(\lambda\)-Stein pair if \((W, W')\) is exchangeable and satisfy the ‘linearity’ or ‘linear regression’ condition

\[
E(W' | W) = (1 - \lambda)W \quad \text{for some} \ \lambda \in (0, 1).
\]
Linearity Condition: Bivariate Normal Connection

Parallel to a property of bivariate normal variables $Z_1, Z_2$: conditional expectation of $Z_1$ given $Z_2$ is linear

$$E(Z_1|Z_2) = \mu_1 + \sigma_1 \rho \left( \frac{Z_2 - \mu_2}{\sigma_2} \right).$$

When $Z_1$ and $Z_2$ have mean zero and equal variance,

$$E(Z_1|Z_2) = (1 - \lambda)Z_2 \quad \text{for } \lambda = 1 - \rho.$$
Linearity Condition: Generator Connection

\[ E(W'|W) = (1 - \lambda)W \quad \text{or} \quad E(W' - W|W) = -\lambda W. \]

Embed in a sequence, \( E(W_{t+1} - W_t|W_t) = -\lambda W_t, \)

\[ \Delta W_t = -\lambda W_t + \epsilon_t \quad \text{where} \ E[\epsilon_t|W_t] = 0. \]

Reminiscent of Ornstein Uhlenbeck process

\[ dW_t = -\lambda W_t + \sigma dB_t. \]
Linearity Condition: Reversible Markov Chain Connection

If $W_1, W_2, \ldots$ is a reversible Markov Chain in stationarity, then $(W_t, W_{t+1})$ is exchangeable.

To apply the method for a given distribution $W$, construct a reversible Markov chain with stationary distribution $W$. 
Anti-Voter Model

On the graph $(\mathcal{V}, \mathcal{E})$, with $|\mathcal{V}| = n$, consider the evolution of the state $\mathbf{X}_t \in \{-1, 1\}^n$ where at each time step a vertex chosen uniformly at random chooses a neighbor at random and adopts the opposite state.

Though $\mathbf{X}_t$ is not reversible, if stationary and the function $W$ satisfies $W(\mathbf{X}_{t+1}) - W(\mathbf{X}_t) \in \{-1, 0, 1\}$ then $(W(\mathbf{X}_t), W(\mathbf{X}_{t+1}))$ is exchangeable.

[Liggett (1985), Rinott and Rotar (1997)]
Let $T$ denote the number of vertices $i$ with $X_i = 1$, and let $U = 2T - n$. Further, let $a, b$ and $c$ be the number of edges whose vertices agree with 1, $-1$, or disagree, respectively.

Observe that for a regular graph of degree $r$

$$T = \frac{2a + c}{r}, \quad n - T = \frac{2b + c}{r}.$$ 

$$P(U' - U = -2 \mid X) = \frac{2a}{rn}, \quad P(U' - U = 2 \mid X) = \frac{2b}{rn}.$$ 

Therefore, using $a + b + c = rn/2$,

$$E[(U' - U) \mid X] = \frac{4b - 4a}{rn} = \frac{2(n - 2T)}{n} = -\frac{2U}{n}.$$
Stein Exchangeable Pair: Mean

When expectations exist they must equal zero, as

\[ EW = EW' = E(E(W'|W)) = E(1 - \lambda)W = (1 - \lambda)EW. \]

As \( 1 - \lambda \neq 0 \),

\[ EW = 0. \]
Stein Exchangeable Pair: Variance Identity

\[ E[W'W] = E(E(W'W|W)) \]
\[ = E(WE(W'|W)) \]
\[ = (1 - \lambda)E(W^2) \]
\[ = (1 - \lambda)\sigma^2 \]

gives

\[ E(W' - W)^2 = 2(EW^2 - EW'W) \]
\[ = 2(\sigma^2 - (1 - \lambda)\sigma^2) \]
\[ = 2\lambda\sigma^2. \]
Stein Exchangeable Pair: Function Identity

Linearity condition gives

\[ E[W'f(W)] = E[f(W)E(W'|W)] = (1 - \lambda)E[Wf(W)], \]

so

\[ E(W' - W)(f(W') - f(W)) = 2E(Wf(W) - W'f(W)) = 2\lambda E[Wf(W)] \]

or

\[ E[Wf(W)] = \frac{E(W' - W)(f(W') - f(W))}{2\lambda}. \]
Exchangeable Pair and the Stein Equation

If \( W, W' \) is Stein pair with variance 1, then

\[
E \left( \frac{(W' - W)(f(W') - f(W))}{2\lambda} \right) = E[Wf(W)].
\]

Taylor expansion

\[
f(W') - f(W) = (W' - W)f'(W) + \int_{W}^{W'} (W' - s)f''(s)ds.
\]

Multiplying by \((W' - W)/(2\lambda)\) results in two terms, the first of which is

\[
\frac{1}{2\lambda} (W' - W)^2 f'(W).
\]
First term of the difference $f'(W) - W f(W)$ is

$$E \left( f'(W) \left[ 1 - \frac{(W' - W)^2}{2\lambda} \right] \right)$$

Since $E(W' - W)^2/(2\lambda) = 1$, conditioning on $W$, applying the Cauchy Schwarz inequality and that $\|f'\|_{\infty} \leq 4\|h\|_{\infty}$ yields the bound

$$R_1 = \frac{2\|h\|_{\infty}}{\lambda} \sqrt{\text{Var}(E((W' - W)^2|W))}.$$
Exchangeable Pair: Second Term

Expectation of

\[ \frac{1}{2\lambda} |(W' - W) \int_W^{W'} (W' - s)f''(s)| \leq \frac{1}{4\lambda} \|f''\|_{\infty} |W' - W|^3 \]

so, applying the bound \( \|f''\|_{\infty} \leq 2\|h'\|_{\infty} \), the second term is bounded by

\[ R_2 = \frac{\|h'\|_{\infty}}{2\lambda} E|W' - W|^3. \]
Let $h$ be bounded and have bounded derivative, and let $W, W'$ be a mean zero, variance 1, $\lambda$-Stein pair. Then

$$|Eh(W) - Nh| \leq R_1 + R_2$$

where

$$R_1 = \frac{2\|h\|_{\infty}}{\lambda} \sqrt{\text{Var}(E((W' - W)^2|W))}$$

and

$$R_2 = \frac{\|h'\|_{\infty}}{2\lambda} E|W' - W|^3.$$
Exchangeable Pair: Example

Let $\pi$ be uniform over $\Pi_n \subset S_n$, the collection of fixed point free ($\pi(i) \neq i$) involutions ($\pi^2(i) = i$) of $\{1, \ldots, n\}$. Special case of a distribution on $S_n$ constant on cycle type, that is, one satisfying

$$P(\pi) = P(\rho^{-1}\pi\rho) \quad \text{for all } \pi, \rho \in S_n.$$ 

Let $\{a_{ij}\}_{i,j}$ be a collection of $n^2$ real numbers. Approximate the distribution of

$$W = \sum_{i=1}^{n} a_{i,\pi(i)}.$$ 

May assume $a_{ij} = a_{ji}$ and $a_{ii} = 0$ without loss of generality.
Let for $a, b, c$ distinct, let $A = \{\pi : \pi(a) = c\}$, and $B = \{\pi : \pi(b) = c\}$, and let $\tau_{ab}$ be the transposition of $a$ and $b$. Then

$$\pi \in A \text{ if and only if } \tau_{ab}^{-1}\pi\tau_{ab} \in B$$

so $P(A) = P(\tau_{ab}^{-1}A\tau_{ab}) = P(B)$ and therefore

$$Ea_{i,\pi(i)} = \frac{1}{n-1} \sum_{j \neq i} a_{i,j} = \frac{1}{n-1} \sum_{j=1}^{n} a_{i,j}.$$  

When considering $\mathcal{L}((W - EW)/\sigma_W)$ we may assume $\sum_j a_{i,j} = 0$ for all $i$ without loss of generality.
Let $I, J$ with $I \neq J$ be chosen uniformly from $\{1, \ldots, n\}$, and set

$$\pi' = \pi \alpha_{IJ}$$

where

$$\alpha_{ij} = \tau_{i, \pi(j)} \tau_{j, \pi(i)}.$$

For $\pi \in \Pi_n$ and $i \neq j$, whereas $\pi$ has the cycle(s)

$$(i, \pi(i)), (j, \pi(j))$$

$\pi'$ has the cycle(s)

$$(i, j), (\pi(i), \pi(j)).$$
Recalling \( W = \sum_i a_{i,\pi(i)} \) and letting \( W' = \sum_i a_{i,\pi'(i)} \), we have

\[
W' - W = 2 \left( a_{I,J} + a_{\pi(I),\pi(J)} - (a_{I,\pi(I)} + a_{J,\pi(J)}) \right).
\]

\[
E[a_{I,J}|\pi] = E[a_{I,J}] = \frac{1}{n(n-1)} \sum_{i,j} a_{ij} = 0
\]

and

\[
E[a_{I,\pi(I)}|\pi] = \frac{1}{n} \sum_{i=1}^{n} a_{i,\pi(i)} = \frac{1}{n} W,
\]

and so, since the resulting expression is \( W \) measurable,

\[
E[W'|W] = (1 - \frac{4}{n})W.
\]
Involutions: Calculating the Bound

Need to compute

$$R_1 = \frac{2||h||_\infty}{\lambda} \sqrt{\text{Var}(E((W' - W)^2|W))}$$

and

$$R_2 = \frac{||h'||_\infty}{2\lambda} E|W' - W|^3$$

for

$$W' - W = 2 \left(a_{I,J} + a_{\pi(I),\pi(J)} - (a_{I,\pi(I)} + a_{J,\pi(J)})\right).$$

Under the usual asymptotic $R_2 = O(n^{-1/2})$. 
Recall

\[ W' - W = 2 \left( a_{I,J} + a_{\pi(I),\pi(J)} - (a_{I,\pi(I)} + a_{J,\pi(J)}) \right). \]

To show \( R_1 = O(n^{-1/2}) \) use

\[ \text{Var}(E((W' - W)^2|W)) \leq \text{Var}(E((W' - W)^2|\pi)). \]

Requires calculation of the variance of a sum of terms such as

\[ E(a_{I,\pi(I)}^2|\pi) = \frac{1}{n} \sum_{i=1}^{n} a_{i,\pi(i)}^2. \]
Zero Bias Coupling

[Goldstein and Reinert (1997)]

Stein identity: \( Z \sim \mathcal{N}(0, \sigma^2) \) if and only if

\[
E[Z f(Z)] = \sigma^2 E[f'(Z)] \quad \text{for all smooth } f.
\]

For any mean zero, variance \( \sigma^2 \) distribution \( \mathcal{L}(W) \) there exists \( \mathcal{L}(W^*) \) satisfying

\[
E[W f(W)] = \sigma^2 E[f'(W^*)].
\]

Distributional transformation \( W \rightarrow W^* \), of which \( \mathcal{N}(0, \sigma^2) \) is the unique fixed point.

Absolutely continuous, \( \text{support}(W^*) \subset \text{co}(\text{support}(W)) \).
Density of $W^*$ is given by

$$p^*(t) = \frac{E[X; X > t]}{\sigma^2}.$$ 

Distribution can also be specified as ‘square biasing’ followed by multiplication by an independent uniform,

$$X^* =_d UX$$

where

$$\frac{dF_Y}{dF_X} = \frac{x^2}{\sigma^2}.$$
Fixed Point Proximity

If $W$ is close to $W^*$, then $W$ is close to being a fixed point of the zero bias transformation, so close to the unique fixed point, so close to normal.
Parallel to the size biasing: If $X_1, \ldots, X_n$ are independent nonnegative (mean zero) random variables with finite nonzero mean (variance), then

$$W = \sum_{i=1}^{n} X_i$$

can be size (zero) biased by replacing a single summand, chosen with probability proportional to its mean (variance) and replacing it with an independent random variable having that summands size (zero) biased distribution, e.g.

$$W^* - W = X_{I}^* - X_{I}.$$
Zero Bias Rationale for CLT

When $W$ is the sum of many comparable variables, $W^*$ differs from $W$ by only a single summand. Hence the distributions of $W$ and $W^*$ are close, so $\mathcal{L}(W)$ is close to being a fixed point of the zero bias transformation, and so must be close to the normal.

One way to make this statement precise is with the following $L^1$ bound: For any coupling of $W$, having variance 1, to $W^*$,

$$||\mathcal{L}(W) - \mathcal{L}(Z)||_1 \leq 2E|W^* - W|.$$
Proof of $L^1$ Bound

Let $W^*$ have the $W$-zero bias distribution, and be defined on the same space as $W$. Then when $\|h'\|_{\infty} \leq 1$,

$$
|Eh(W) - Nh| = |E[f'(W) - Wf(W)]| \\
= |Ef'(W) - Ef'(W^*)| \\
\leq \|f''\|_{\infty} E|W - W^*| \\
\leq 2\|h'\|_{\infty} E|W - W^*| \\
\leq 2E|W^* - W|.
$$

Taking supremum over all $h$ with $\|h'\|_{\infty} \leq 1$ yields

$$
\|\mathcal{L}(W) - \mathcal{L}(Z)\|_1 \leq 2E|W^* - W|.
$$
If \( dF(w', w'') \) is the distribution of the Stein pair \( W', W'' \) let \( W^\dagger, W^\ddagger \) have distribution

\[
dF^\dagger(w', w'') = \frac{(w' - w'')^2}{2\lambda\sigma^2} dF(w', w'').
\]

Then if \( U \) is a uniform variable, independent of \( W^\dagger, W^\ddagger \),

\[
W^* = UW^\dagger + (1 - U)W^\ddagger
\]

has the \( W \)-zero biased distribution.
Let $\mathbf{Y} = (Y_1, \ldots, Y_n) = \text{d} (\pm Y_1, \ldots, \pm Y_n)$ with $\text{Var}(Y_i) = \sigma_i^2 \in (0, \infty)$ and $W = \sum_{i=1}^n Y_i$. Let $Y^i \sim y_i^2 dF(y)/\sigma_i^2$, $I$ a random index independent of $\mathbf{Y}$ and $\{Y^i, i = 1, \ldots, n\}$ with distribution

$$P(I = i) = \frac{\sigma_i^2}{\sum_{j=1}^n \sigma_j^2},$$

and $U \sim \mathcal{U}[-1, 1]$ independent of all other variables. Then

$$W^* = U Y_I^I + \sum_{j \neq I} Y^I_j$$

has the $W$-zero bias distribution.
Connection to $K$ function

For a mean zero random variable $X$, Chen and Shao let

$$K(t) = E(X1_{0 \leq t \leq X} - X1_{X \leq t < 0}) = E(X1_{X > t}) \quad \text{a.e.,}$$

so $K(t)/\sigma^2$ is the zero bias density. For a sum $W$ of independent variables, letting $W = W^{(i)} + X_i$, they write

$$E[Wf(W)] = \sum_{i=1}^{n} \int_{-\infty}^{\infty} E[f'(W^{(i)} + t)] K_i(t) dt,$$

which is $\sigma^2 Ef'(W^*)$, as the expression above equals

$$\sigma^2 \sum_{i=1}^{n} \frac{\sigma_i^2}{\sigma^2} \int_{-\infty}^{\infty} E[f'(W^{(i)} + t)] \frac{K_i(t)}{\sigma_i^2} dt = \sigma^2 Ef'(W_I + X_I^*).$$
Comparison of three couplings

1. Exchangeable pair: linearity condition, evaluation of the variance of a conditional expectation.

2. Size bias: no linearity condition, evaluation of the variance of a conditional expectation.

3. Zero bias:
   (a) Construction through exchangeable pair: linearity condition, no variance of conditional expectation.
   (b) Construction through square biasing: symmetry condition, no variance of conditional expectation.
IV. Local dependence, Nonsmooth functions